



ABOUT CHEMICAL TRENDS IN TRANSITION METAL COMPLEXES

ÜBER CHEMISCHE TRENDS IN ÜBERGANGSMETALLKOMPLEXEN

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*„What we observe is not nature itself,
but nature exposed to our method of questioning.“*

WERNER HEISENBERG

Abstract

The present doctoral thesis developed around the objective to generate a bench-stable electrophilic fluorinating reagent (like Selectfluor¹) from inorganic fluoride as fluorine source. In contrast to the preceding Master's thesis,^[1] this thesis does not focus on the synthesis and analysis of potential complexes to catalyze the aforementioned reaction, but rather on some of the theoretical vacancies that deter us as a scientific community from understanding what to take care of in order to successfully design such a reaction.

This thesis presents another fraction of this groundwork like the analysis of an electrophilic fluorination reaction mechanism from a high-valent palladium fluoride complex, the non-existence of a potential "Fluoro Wall" (the respective fluoro-analogue of the Oxo Wall), the generation of a novel all-electron basis set to accurately calculate relativistic properties of fifth period elements, and of course the parallel developments in computational catalyst design for the oxidative activation of fluoride.

Zusammenfassung

Die vorliegende Doktorarbeit entwickelte sich um das Ziel, ein "tischstabiles"² elektrophiles Fluorierungsreagenz (wie Selectfluor) aus anorganischem Fluorid als Fluorquelle zu synthetisieren. Im Gegensatz zur vorhergehenden Masterarbeit^[1] konzentriert sich diese Arbeit nicht auf die Synthese und Analyse potentieller Komplexe zur Katalyse der oben erwähnten Reaktion, sondern auf einige der offenen theoretischen Fragestellungen, die uns als wissenschaftliche Gemeinschaft davon abhalten zu verstehen, worauf wir achten müssen, um eine solche Reaktion erfolgreich zu gestalten.

In dieser Arbeit wird ein weiterer Bruchteil dieser Grundlagenarbeiten vorgestellt, wie die Analyse eines elektrophilen Fluorierungsreaktionsmechanismus aus einem hochvalenten Palladiumfluoridkomplex, die Nichtexistenz der „Fluoro Wall“ (das entsprechende Fluor-Analogon zur Oxo Wall), die Generierung eines neuartigen Vollelektronenbasissatzes zur genauen Berechnung der relativistischen Eigenschaften von Elementen der fünften Periode und natürlich die parallelen Entwicklungen bei dem computergestützten Entwurf von Katalysatoren für die oxidative Aktivierung von Fluorid.

¹Within this thesis, the term "F-TEDA" is regularly used to describe the Selectfluor dication, and the term "TEDA" (derived from "Tetraethylenediamine", synonymous for the DABCO backbone of the Selectfluor structure) for the corresponding defluorinated cation.

²„Tischstabil“ in diesem Zusammenhang bedeutet, dass der betreffende Stoff ohne besondere Vorkehrungen auf einem Labortisch gelagert werden kann.

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First, I want to thank PROF. DR. FRANK NEESE for giving me the opportunity to join his research group, for his support and for the beautiful freedom regarding my research projects. I honestly could not have asked for a better supervisor in any respect.

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I dedicate this thesis to my incredible and supportive family (including those I've consciously chosen to be part of it)³ for all they have done for me. I am nothing without you. This thesis belongs to all of us.

³If you read this thesis for correction, definitely consider yourself part of it!

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Abbreviations

AO	atomic orbital
CC	Coupled Cluster
cf.	confer
CI	Configuration Interaction
CPCM	Conductor-like Polarizable Continuum Model
D	double substitutions
DFT	Density Functional Theory
DLPNO	Domain-based Local Pair Natural Orbital
e. g.	for example (<i>exempli gratia</i>)
ECP	Effective Core Potential
F-TEDA	Selectfluor dication (IUPAC: 1-chloromethyl-4-fluoro-1,4-diaza-bicyclo[2.2.2]octane dication)
GGA	Generalized Gradient Approximation
GTO	GAUSSIAN-type orbitals
HF	HARTREE-FOCK
HOMO	highest occupied molecular orbital
i. e.	that is (<i>it est</i>)
incl.	including
LDA	Local Density Approximation
LUMO	lowest unoccupied molecular orbital
MO	molecular orbital
PES	Potential Energy Surface
PET	Positron Emission Tomography
PP	pseudopotential
QRO	quasi-restricted orbital
RI	Resolution of Identity Approximation
S	single substitutions
SARC	Segmented All-Electron Relativistically Contracted
SCF	self-consistent field
SET	single-electron transfer
SOMO	singly occupied molecular orbital

SPP	Spin Polarization Parameter
STO	SLATER-type orbital
T	triple substitutions
TEDA	1-chloromethyl-1,4-diazabicyclo[2.2.2]octane cation
UCO	unrestricted corresponding orbitals
ZPE	zero-point vibrational energy

1 Introduction

The present work focuses on the theoretical evaluation of experimentally observable trends in transition metal complexes. A vast majority of this work deals with computational analyses of reactivity patterns of late transition metal fluoride complexes with a focus on and around high-valent monofluoride complexes of group 10 elements (Ni, Pd, Pt).

In this first chapter, the chemical and methodological groundwork is reviewed, before the present research objective and methodology are described in more detail in the next. In chapter 3, the scientific advances^{[2]–[4]} of my research are presented and contextualized, before the general “Train of Thought” of the studies, on which this doctoral thesis is grounded, is discussed in some more detail. The thesis is finally summarized in chapter 4.

1.1 Preface

This thesis is supposed to comprehend the scientific advances I contributed to during the last four years. However, it would be totally inaccurate to boil down my doctoral phase to my scientific advances only. Looking back, this phase is probably also the time of my life – at least so far – I grew the most not only as a scientist, but also as a person. This is why I decided to append not only my scientific, “academic publications”, but also what I call my “other publications” (at least the ones that were published in written form) from this time: to start this thesis as a person⁴ *and* to end it as such.

I hope you enjoy reading it.

⁴As opposed to the pure and dry function of a scientist with the aspiration of (pseudo-)objectivity.

1.2 Chemical Groundwork

Chemically, the work presented here builds on two major fundamentals: The first one is the concept of the so-called “Oxo Wall” and the second is the recent advance in synthetic and catalytic applications of (high-valent) late transition metal fluoride complexes, especially palladium fluorides:

1.2.1 The Oxo Wall⁵

The Oxo Wall is a widely known and accepted concept among the inorganic chemical community.^[5] It states the instability of six-coordinate tetragonal oxo complexes with metals beyond group 8.

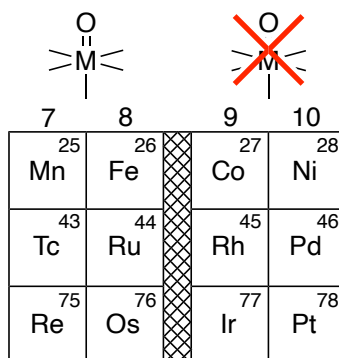


Figure 1: Depiction of the Oxo Wall.

While transition metal oxo complexes are a prominent motif in biological oxidation processes,^{[6],[7]} the concept of the Oxo Wall dates back to 1962 where BALLHAUSEN and GRAY developed a molecular orbital energy level scheme that correctly described the electronic structure of the vanadyl ion.^[8] The description of chromyl and molybdenyl ions followed shortly after, where the metal oxo interaction was represented as a triple bond for the first time.^[9]

This notion is based on elementary molecular orbital considerations in which the bond order is deduced by subtracting the number of electrons in antibonding orbitals of a given bond from the number of electrons in the bonding counterparts of these orbitals and divide the result by two.^[10] For example, in the six-coordinate tetragonal oxo complex Mo(V)OCl_5^{2-} the single d electron is found in the nonbonding d_{xy} orbital, leaving the two other d orbitals of t_{2g} symmetry (d_{xz} and d_{yz}) amenable to π interactions with the $p_{x/y}$ orbitals from the oxo ligand on the z axis. A total of six electrons are present in the two bonding π -orbitals and the bonding σ -orbital (interaction between oxo p_z and metal d_{d^2} orbital) while all antibonding counterparts are empty, thus leaving a metal-oxo triple bond.

The theoretical concept of the Oxo Wall – as stated by GRAY and WINKLER: “Complexes with tetragonal symmetry can have no more than 5 d electrons and still retain some MO multiple

⁵This subchapter is copied from the Manuscript “Where Is the Fluoro Wall?: A Quantum Chemical Investigation”^[3] that will be presented and discussed in the course of this work.

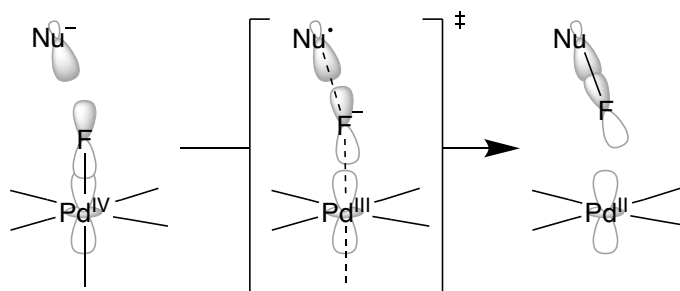
bonding. In the absence of π -bonding to the metal, the oxo will be extremely basic and unstable with respect to protonation or attack by electrophiles.”^[5] – is also supported by a large array of experimental investigations.^{[11]–[13]} While oxo compounds are known with transition metals beyond the Oxo Wall^{[14],[15]} with well-characterized electronic structure,^[16] these do not violate the concept of the Oxo Wall because they are not of tetragonal symmetry. Claims that exceptions have been found^[17] were later retracted and as such, ‘the “Oxo Wall” stands.’^[18]

1.2.2 (High-Valent) Late Transition Metal Fluorides

Transition metal fluorides are known and used for many decades.^{[19],[20]} They are readily accessed via oxidative C–F bond activation,^[21] nucleophilic fluorination^[22] or oxidative electrophilic fluorination.^[23] Despite the fact that the range of natural organofluorine compounds is very limited,^[24] fluorinated molecules are of particularly high interest in materials, agrochemicals and pharmaceuticals.^{[25]–[31]} Especially the emergence of Positron Emission Tomography (PET)^[32] and the concomitant need for late-stage fluorination methodologies to effectively include the radioisotope ^{18}F into organic molecules gave rise to a totally new form of reaction design, the so called “radiofluorination”.^{[33]–[37]}

Especially important for this work are those late transition metal fluoro complexes that would violate a potential Fluoro Wall, the fluoro equivalent to the well documented Oxo (cf. 1) and Nitro Walls^{[38],[39]}; in contrast to the latter elements, even perfectly octahedral hexafluoride complexes beyond the potential Fluoro Wall are well documented.^[40] Furthermore, fluoro complexes with six-coordinate tetragonal geometry for a significant part of the second half of the transition metals are often hypothesized (with varying degrees of evidence) as active intermediates in catalytic fluorination reactions.^[25]

A big step forward was the experimental revelation that, shown with a cationic palladium fluoride,^[41] high-valent late transition metal fluoride complexes can in principle serve as $\text{S}_{\text{N}}2$ “fluoronium” (F^+) donors. This means, starting from fluoride, the compound mentioned above is able to perform an *umpolung*-like reaction^[42] on fluorine, the most electronegative element of the periodic table. Interestingly, it has been shown that this $\text{S}_{\text{N}}2$ -type “fluoronium” transfer proceeds through an unusual SET/fluoride transfer/SET mechanism:^[43] instead of transferring an F^+ , after all, the fluorine is transferred in the form of an F^- , enclosed by two individual single-electron transfers (SET) from the nucleophile to the palladium. Hence, this reaction type is more accurately described as an oxidative fluorination.



Scheme 1: $\text{S}_{\text{N}}2$ -type fluorination reaction, following an unusual SET/fluoride transfer/SET mechanism.

1.3 Methodological Groundwork⁶

As the present work is mostly theoretical, the following part seeks to introduce the basic theories behind the field of computational chemistry. The main objective of computational chemistry is to accurately describe intrinsic properties of a chemical system by means of quantum mechanical methodology. There are different strategies to approach the quantum physical description of a given chemical system, with the two most prominent being electron-wave-function-based on the one hand and electron-density-based on the other hand.

1.3.1 *Ab initio* Methods: Hartree-Fock and Beyond

The family of *ab initio* methods generally tries to solve the (time independent) SCHRÖDINGER equation:^[44]

$$\hat{H}|\psi\rangle = E|\psi\rangle \quad (1)$$

$\hat{H}$: HAMILTONIAN

$|\psi\rangle$: Vector notation of an n dimensional wave function

E : Energy eigenvalue of the wave function $|\psi\rangle$

For molecular systems, the HAMILTONIAN, the operator corresponding to the sum of all kinetic plus potential energies of all particles in a given system, generally takes the following form:

$$\hat{H} = \hat{T}_e + \hat{V}_{Ce} + \hat{V}_{ee} \quad (2)$$

$\hat{T}_e$: Operator of the kinetic energy of the electrons

$\hat{V}_{Ce}$: Operator of the potential energy of the core electron attraction

$\hat{V}_{ee}$: Operator of the potential energy of the electron electron repulsion

In quantum chemical systems, the nuclei are generally assumed to be stationary (BORN-OPPENHEIMER approximation).^[45] Hence, the kinetic energy of the nuclei ($\hat{T}_C$) is neglected in the above description of the HAMILTONIAN. Also, the wave function is reduced to the description of the electronic configuration. Because of this, the family of *ab initio* methods can be considered as electron-wave-function-based approaches.

In principle, the solutions of the SCHRÖDINGER equation include the whole field of solid state physics and chemistry (neglecting relativistic effects). However, exact solutions exist only for one-electron systems like the hydrogen atom. For anything beyond, numerical techniques are required to approximate the interelectronic interactions.

Hartree-Fock Method The HARTREE-FOCK method^{[46]-[48]} (HF) simplifies these interactions by describing the multi-electron wave function through a SLATER determinant. As a result,

⁶There is a certain similarity between this subchapter and a comparable subchapter in my Master's thesis.^[1]

the individual electrons no longer interact in pairs, but with a field of all other particles in the so-called “mean field”. The field still depends on the behaviour of the individual particles, but the solution can now be calculated gradually:

First, an initial state is selected from which the mean field is generated. Using this field, the SCHRÖDINGER equation is then solved for each individual particle. Together, the individual solutions then result in a new state and a new field. This process is repeated until successive solutions differ only slightly, resulting in a self-consistent field (SCF), i.e. the field leads to solutions that consistently generate the field itself again.

The systematic error, generated by neglecting the exact interaction of the electrons with each other, is called “electron correlation”.

Post-Hartree-Fock Methods Building up on HF, various methods that are able to capture at least certain parts of the electron correlation have been developed. Of particular importance are the Configuration Interaction (CI)^{[49],[50]} and Coupled Cluster (CC)^{[51]–[53]} methods as well as the MØLLER-PLESSET (MP) perturbation theory^{[54],[55]}, which are all based on the solution of the HARTREE-FOCK method.

While inclusion of electron correlation generally drastically increases the accuracy of the calculations, one has to consider that especially for larger chemical systems, the computing time of these methods can easily exceed a human life time. Practically, quantum mechanical calculations of chemical systems are subjected to a compromise of accuracy and time, thus the choice of the calculational method is based on a constant trade-off between the best accuracy possible and a reasonable time scale to complete the calculation.

Arguably a “quantum step” forward was the recent development of the (linearly scaling) Domain-based Local Pair Natural Orbital Coupled Cluster (DLPNO-CC)^[56] method. Including single, double and perturbed triple excitations, DLPNO-CCSD(T) recovers more than 99.9 % of the correlation energy of CCSD(T)^[58] – which is often considered the gold-standard of computational chemistry^[57] – while only taking twice to four times as long as a standard DFT calculation on the same system.^[59]

Multi-Reference Methods A second important development from the HARTREE-FOCK method are multi-reference methods like the Complete Active Space Self-Consistent Field (CASSCF)^{[60]–[62]} or the n-Electron Valence Perturbation Theory (NEVPT)^{[63]–[65]} method. In contrast to the single-reference methods, these methods use linear combinations of multiple determinants in order to describe states that are not accurately calculated with a single determinant like e. g. (quasi-)degenerate ground states, low excitation states or bond breaking.

1.3.2 Density Functional Theory

Density Functional Theory (DFT) is a method to evaluate the energy of an N electron system without the complete solution of the SCHRÖDINGER equation by calculating the ground state

energy via the electron density ρ , which describes the system completely. One could say, instead of building up the wave function from scratch by trying to simulate the electrons one by one, one rather looks at the complete picture it draws. The advantage of this alternative compared to wave function based methods is the reduction of the necessary coordinates from $3N$ to 3.⁷

The (spin free) electron density can be considered as the probability of the presence of one of N electrons in the voxel $d\vec{r}$ and is calculated by integrating the square of the N -electron wave function's absolute value over $N - 1$ electron coordinates as well as N electron spins:

$$\rho(\vec{r}) = \rho(\vec{r}_1) = N \int \cdots \int |\psi(x_1, x_2, \dots, x_N)|^2 ds_1 dx_2 \dots dx_N \quad (3)$$

The first HOHENBERG-KOHN theorem^[66] states that the ground state energy $E_e[\rho]$ can be expressed as a functional of the ground state electron density ρ :

$$E_e[\rho] = \langle \psi | \hat{T}_e + \hat{V}_{Ce} + \hat{V}_{ee} | \psi \rangle = \mathcal{F}^{HK}[\rho] + E_{Ce}[\rho] \quad (4)$$

$\mathcal{F}^{HK}$: HOHENBERG-KOHN functional

E_{Ce} : Potential energy of the core electron attraction

Since $\hat{T}_e$ and $\hat{V}_{ee}$ only depend on the electron coordinates $\vec{r}$, their observables can be condensed to the functional $\mathcal{F}^{HK}$. $\mathcal{F}^{HK}$ then only depends on N which can easily be calculated by integrating $\rho(\vec{r})$ over the complete space:

$$\int \rho(\vec{r}) d\vec{r} = N \quad (5)$$

$\hat{V}_{Ce}$ however depends further on the core coordinates $\vec{r}_A$ as well as core charges Z_A . The number of cores M as well as $\vec{r}_A$ can be extracted from the maxima of $\rho(\vec{r})$ and Z_A through derivation of $\rho(\vec{r})$ at the core coordinates. This makes $\hat{V}_{Ce}$ dependent on the exact form of $\rho(\vec{r})$.

The second HOHENBERG-KOHN theorem states that $E_e[\rho]$ is variational ($\tilde{E}_0 \geq E_0$) which means that the electron density ρ can be achieved by systematical minimization of $E_e[\rho]$ through variation with eq. 5 as secondary condition, at least in principle.

The major problem of this method is the fact that the HOHENBERG-KOHN functional $\mathcal{F}^{HK}$ is unknown and has to be approximated. This means, the accuracy of $E_e[\rho]$ is directly dependent on the accuracy of the approximation of $\mathcal{F}^{HK}$. To minimize the error, KOHN and SHAM divided the HOHENBERG-KOHN functional $\mathcal{F}^{HK}$ into the non correlating kinetic energy T_0^{KS} , the electron electron repulsion J^{KS} and the exchange/correlation functional E_{XC} .^[67] The latter contains all unknown values and can be approximated by different methods:

Local Density Approximation (LDA). The basis of the LDA is the theory of the homogenous electron gas. E_{XC} is described as a function of the electron density ρ at the observed coordi-

⁷This is valid for the spin free electron density. Addition of the spin information leads to the addition of one further dimension.

nate. Through this approximation the exchange/correlation functional E_{XC} of a system with consistent electron density can be determined relatively accurately.

Generalized Gradient Approximation (GGA). Compared to the LDA, the GGA also considers the gradient of the electron density ρ , i.e. the derivative with respect to the position. This approach describes the inhomogeneities of ρ in atoms and molecules better than LDA. The results of molecule geometries or ground state energies calculated with this method are generally relatively accurate.

Hybrid Approaches. If E_{XC} is calculated by a hybrid method, a part of the exchange energy is calculated via HF, the other part as well as the correlation energy via GGA and/or LDA. The calculated energies finally contribute differently weighted to E_{XC} .^[68]

Though there are multiple methods of a great variety, there is currently no universal method for calculations on organic molecules.^[69] However, for computational investigations – especially into organic and inorganic reactions – DFT has shown to give an adequate compromise between accuracy and speed and is thus the general method of choice.^{[70]–[73]}

1.3.3 Basis Sets

While the choice of the applied method is a major factor contributing to the accuracy of a quantum chemical calculation, another factor – arguably as relevant as the method – that has to be considered is the choice of basis sets. The function of the basis set is to model atomic orbitals (AO) as well as molecular orbitals (MO) by linear combination of basic functions $|\varphi_i\rangle$ which build the basis set:

$$|\psi\rangle = \sum_i^n c_i |\varphi_i\rangle \quad (6)$$

Though SLATER-type orbitals (STO) generally describe the shape of AOs best, GAUSSIAN-type orbitals (GTO) are generally preferred due to their more efficient application.^[74]

Effective Core Potentials (ECP). Since the effect of the chemical environment on the core electrons can often be neglected, effective core potentials (ECP) or pseudopotentials (PP) can be used for a simplified description of the innermost electrons. They approximate the complex description of core electrons, which – especially for heavier atoms – are subject to increasing relativistic effects, through an effective potential. Above a certain cutoff radius r_C , this simplification matches with the complete relativistic description of the core electrons, leading to accurate valence properties despite this approximation.^[68]

All-Electron Basis Sets. However, due to the steady growth of computational resources as well as the improvement of available methods – and moreover, because calculation of properties like X-ray absorption or Mößbauer spectra rely on an accurate (relativistic) description of the innermost core electrons, all-electron basis sets for elements beyond Krypton are increasingly becoming both, accessible and common. For the present work, the “Segmented All-Electron Relativistically Contracted” (SARC) Basis Sets, a set of scalar relativistic all-electron basis sets from the Neese group, should quickly be introduced.^[75] The SARC basis set family follows a design principle in which the GTOs with biggest exponents, representing the innermost shells, are contracted (we could say “frozen”) into a single orbital function, which leads to a significant speedup without relevant loss of accuracy.^{[76]–[81]}

2 Objective and Methodology

The research vacancy that is attempted to be addressed in this thesis is the *umpolung* reaction of fluoride. The overall goal is the synthesis of a bench-stable and at the same time reactive electrophilic fluorinating reagent like *N*-fluorobenzenesulfonimide (NFSI) or F-TEDA, starting from fluoride as fluorine source. Such reaction would e.g. revolutionize the synthetic accessibility of ^{18}F -Tracers in high specific activity for Positron Emission Tomography (PET). The knowledge generated and collected in this thesis is supposed to help achieve this objective in due time.

As this work focusses on the theoretical, quantum chemical analysis of molecular systems and reactions, all of the work presented in here was performed using the ORCA program package.^{[82],[83]} In the following paragraphs, I will introduce my standard setup:

DFT calculations were normally performed with the PBE0 functional^[84] and the def2-TZVP basis set^[85] including GRIMME's D3 dispersion correction with the BECKE-JOHNSON damping scheme.^{[86],[87]} The Resolution of Identity Approximation (RI)^{[88]–[90]} was used for the COULOMB integrals with the def2/J auxiliary basis set^[91] and for the HF exchange terms with the Chain of Spheres Approximation (COSX).^[92]

In general, geometries were either built from scratch using the molecular builder in the Avogadro^[93] program or extracted from a crystal structure, and either way subsequently optimized by DFT. Local minima were confirmed through frequency analysis. Self-consistent field (SCF) and optimization convergence criteria were set tightly (ORCA keywords "TightSCF" and "TightOpt"). Sometimes the integration grid was enlarged (ORCA keyword "Grid6") and convergence problems were mostly solved through employing alternative algorithms like KDIIS or SOSCF. Orbital analyses included quasi-restricted orbitals (QRO)^[94] and unrestricted corresponding orbitals (UCO)^[95] that were called with the ORCA keywords "UNO" and "UCO".

CASSCF calculations generally started from DFT orbitals and geometries with the same basis sets, utilizing TrafoStep RI with the def2/JK auxiliary basis sets^[96] and the AILFT module.^{[97],[98]} SCF convergence criteria were also set tightly.

DLPNO-CCSD(T) calculations generally started from DFT geometries employing the DKH2 scalar-relativistic HAMILTONIAN^{[99]–[105]} and the relativistically recontracted DKH-def2-TZVPP basis sets.^[85] For heavy elements ($Z > 36$), the SARC-DKH-TZVPP basis sets were used.^[76] SCF convergence criteria were also set tightly, auxiliary basis sets were generated on the fly with the AutoAux command^[106] and the Conductor-like Polarizable Continuum Model (CPCM)^[107] was used to simulate implicit solvation in MeCN.

2.1 Representative Input File Headers

- A typical header for ground state geometry optimizations:

```
! PBE0 D3 Opt Freq RIJCOSX def2-TZVP def2/J TightSCF TightOpt
! (Grid6 NoFinalGrid / UNO / UCO / KDIIS / SOSCF)
```

- A typical header for a broken symmetry transition state optimization:

```
! PBE0 D3 OptTS Freq RIJCOSX def2-TZVP def2/J
! TightSCF TightOpt Grid6 NoFinalGrid
%scf brokensym 1,1 end
%geom calc_hess true end
```

- A typical header for a CASSCF calculation:

```
! M0Read def2-TZVP def2/JK TightSCF
%casscf nel 3 norb 5 nroots 10 actorbs dorbs trafostep ri end
%M0Inp "dft_opt.gbw"
```

- A typical header for a DLPNO-CCSD(T) calculation:

```
! DLPNO-CCSD(T) DKH-def2-TZVPP DKH2 AutoAux TightSCF
! CPCM(Acetonitrile)
%basis NewGTO Pt "SARC-DKH-TZVPP" end
NewAuxJGTO Pt "AutoAux" end
NewAuxJKGTO Pt "AutoAux" end
NewAuxCGTO Pt "AutoAux" end end
```


3 Results and Discussion

In this chapter I will present the most important research advances of my doctoral studies and try to set them into context.

3.1 “Palladium–catalysed electrophilic aromatic C–H fluorination”

When I started my doctoral studies in the RITTER group in 2016, we were in the middle of the development (incl. reaction analysis) of a palladium-catalyzed aryl C–H fluorination reaction. Besides some laboratory work (incl. scanning of the substrate scope and mechanistic studies) I was mostly occupied with the computational analysis of the reaction mechanism. As it turned out, the fluorination of the arene, starting from the [Pd(IV)–F] complex, seems to proceed in a similar fashion as the former S_N2 -type oxidative fluorination reaction: after an initial SET from the arene to the metal center, a fluoride anion is transferred, before a second electron is transferred. The corresponding transition state of this fluoride-coupled electron transfer reaction favors a broken spin symmetry solution. In Fig. 2, the resulting magnetic orbital pair is visualized as UCOs for the *para*-fluorination of chlorobenzene.

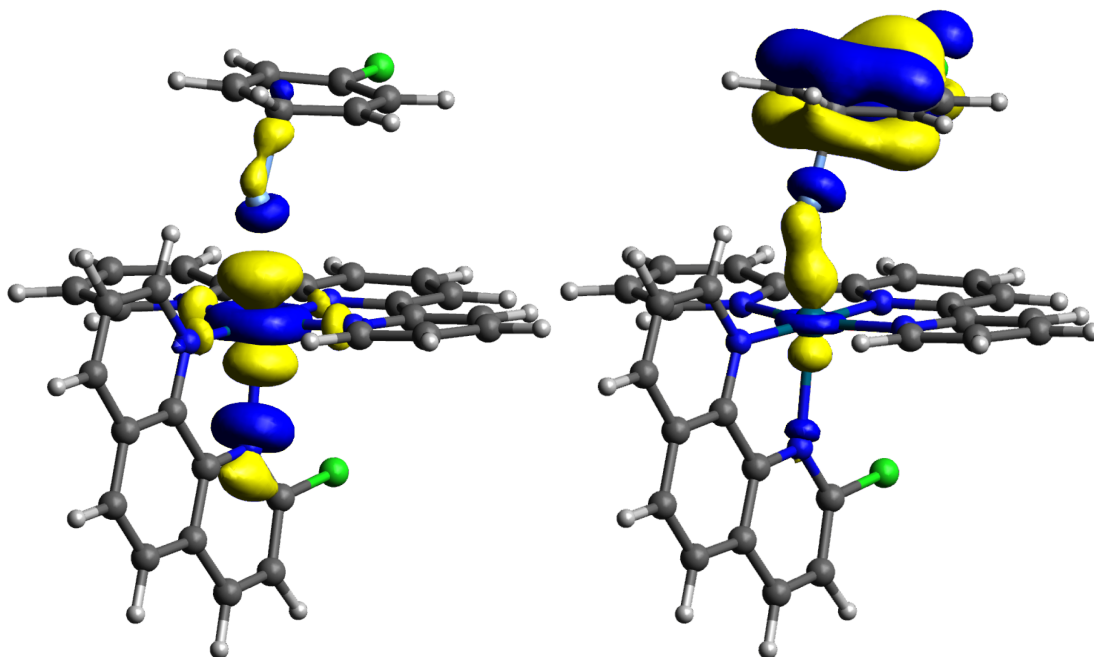


Figure 2: Visualization of the unrestricted corresponding orbitals (UCOs) representing the magnetic orbital pair of the palladium-catalyzed aryl C–H fluorination reaction's transition state: *para*-fluorination of chlorobenzene (left: alpha, right: beta; iso = 0.05).

This showed that the previously described SET/fluoride transfer/SET mechanism is a pattern generalizable to other systems as well – a second palladium fluoride complex that proceeds an oxidative fluorination through a fluoride coupled electron transfer reaction. It's a remarkably rare example for the single-electron reactivity of Pd (as Pd is known to highly prefer even oxidation states).^[108]

The mechanistic analysis was included in the final publication of the reaction (A1.1).^[2]

3.2 “Where Is the Fluoro Wall?: A Quantum Chemical Investigation”

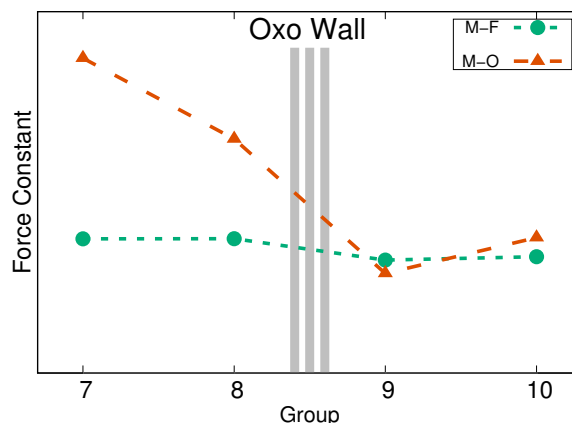


Figure 3: Graphical abstract of the publication “Where Is the Fluoro Wall?: A Quantum Chemical Investigation”.^[3]

After my transition to the NEESE group, my predominant research focus was to find an answer to the question: “Why is there a Nitrido and an Oxo Wall, but apparently no Fluoro Wall?” The long answer is appended (A1.2);^[3] the short answer is: because the additional core charge pushes the $2p$ AO energies of the fluoro ligand too low to meaningfully π -interact with the empty metal d orbitals. For the oxo ligand, in contrast, the $2p$ AO's are energetically close enough to the metal d orbitals to form a proper π bond – or even two (cf. Fig. 4). This, however, comes with the price of extreme reactivity as soon as the d/π^* antibonding orbitals are filled with electrons; six-coordinate tetragonal oxo complexes beyond group 8 are stable *in silico* only.

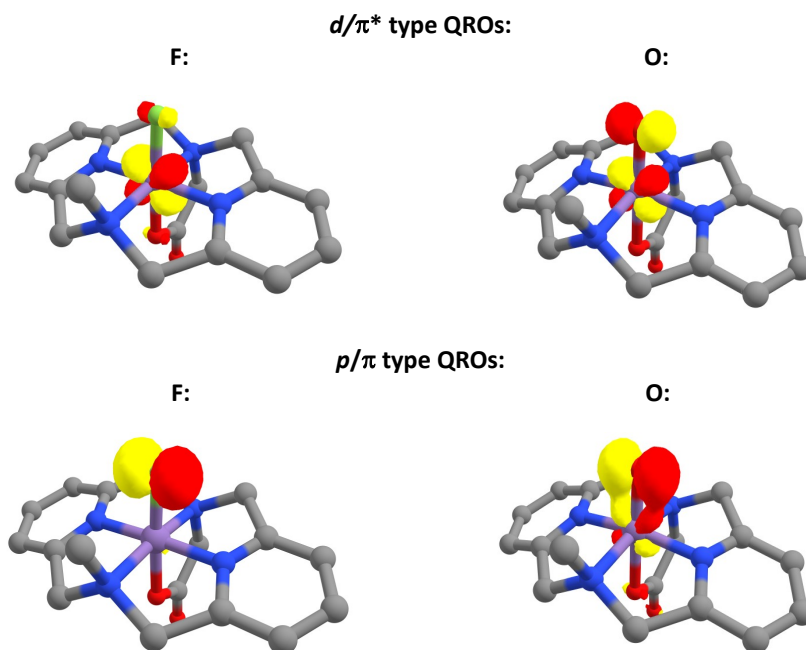


Figure 4: Representative d/π^* (top) and p/π (bottom) QROs for fluoro (left) and oxo (right) complexes (iso = 0.05).

3.3 “All-electron scalar relativistic basis sets for the elements Rb–Xe”

During my work on the computational analysis of several transition metal complexes, I came across the fact that in ORCA’s SARC series of scalar-relativistic all-electron basis sets, no basis sets were provided for the 5th period elements, including the second-row transition metals (4*d* elements). So I developed them with the help of DIMITRIOS PANTAZIS. The corresponding publication is also appended (A1.3).^[4]

We build a basis set in triple- ζ quality (SARC-TZV), consisting of 112 – 115 functions, contracted to 70 – 73 functions:

- (22s15p9d)[15s10p5d] for *s* and *d* block elements (Rb–Cd)
- (22s16p9d)[15s11p5d] for *p* block elements (In–Xe)

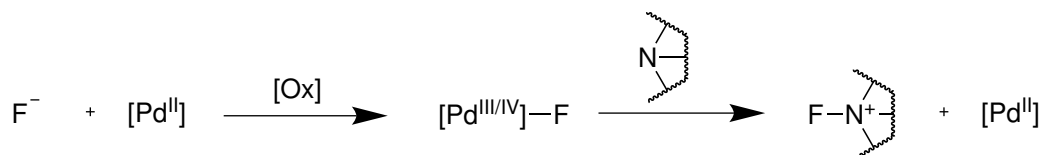
Additionally, we developed a polarization extension for DFT calculations (P), consisting of an additional *f* function for *d* and *p* block elements, and a correlation extension for post-HF methods (PP), consisting of an additional *f* function for *s* block elements, two additional *f* functions for *p* block elements, and one additional *d*, two *f*, and one *g* function(s) for *d* block elements.

3.4 The Train of Thought – Unfinished and Abandoned Ideas

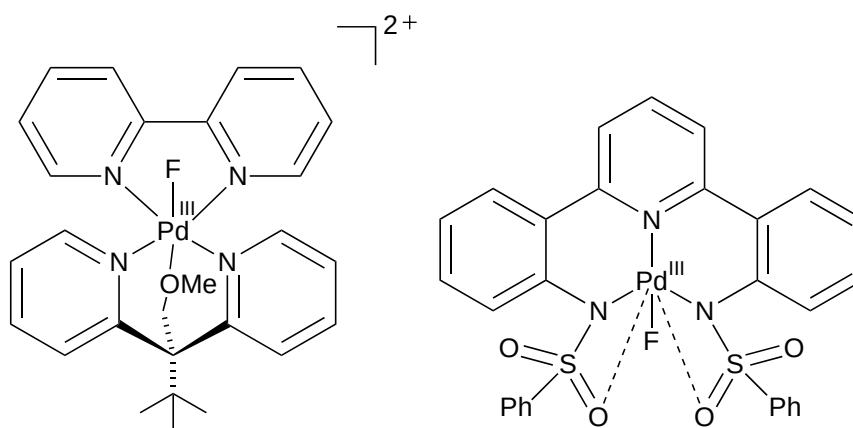
The idea of this subchapter is to discuss those ideas that didn't succeed, but are still found worth being mentioned. The decision to include this chapter into this thesis follows two reasons: on the one hand I don't want this information to be wasted, maybe somebody else will find a fertile soil in these ideas. On the other hand, it's a political move. Our community is obsessed with success stories, with competition, with shining CV's. We rarely talk about things that didn't work, especially when it comes to official publications. I believe, every success story is only complete if it contains some information about the dead ends as well. So here are mine.

3.4.1 "Oxidative Activation of Fluoride for Organic Synthesis" – How It Started

The research objective addressed in Chapter 2 – the *umpolung* reaction of fluoride – started following me when I started my Master's thesis with TOBIAS RITTER.^[1] The whole thesis deals with the synthesis of Pd(III) fluoride complexes that could potentially be able to fluorinate TEDA:



Scheme 2: General depiction of the desired *umpolung* reaction of fluoride.



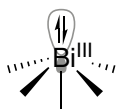
Scheme 3: Proposed complex structures for the reaction depicted in scheme 2.

Of course they didn't work. But that was not the end of the chase. During my doctoral studies, I followed this thought a couple more times into different directions. The overall objective, as given in scheme 2 stayed almost the same – the only change is that I started moving away from Pd as the metal center; I started looking e.g. into fluoride complexes of group 11 elements (Cu, Ag, Au), as well as Ru, Ir, Rh, Rh₂, and other bimetallic fluoride complexes that could electrophilically fluorinate TEDA.

3.4.2 Bismuth – The Next Big Player

At some point I stumbled upon Bismuth. It initially caught my attention due to a hint about the Bi–F bond being quite weak. I didn't find proper data to substantiate this claim, but I still started looking into the electronic structure of Bismuth. I started thinking about bimetallic systems with Pd and Bi, combining their properties, but discontinued that path quite early. Eventually, the reports from our institute by the CORNELLA group regarding Bi-catalyzed aryl fluorination^[109] made me spark up that direction again.

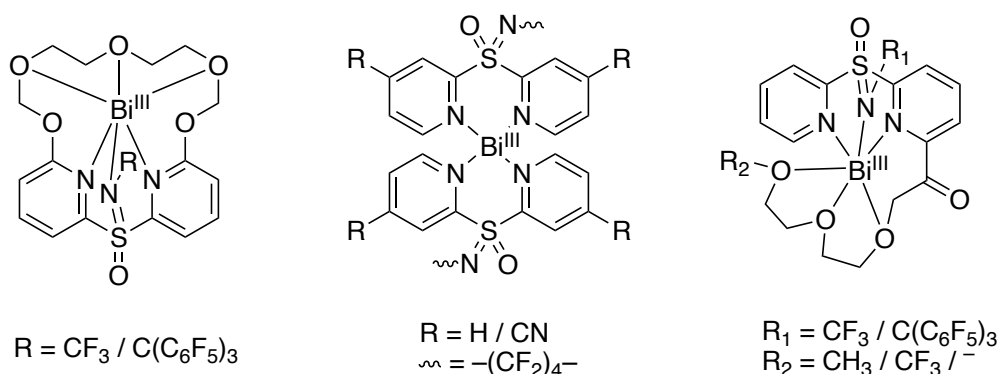
The Bi(III)/(V) redox system has a beautiful and almost unique property – while the electronic system of Bi(V) has a completely empty valence shell, Bi(III) has a lone pair that can be localized in an sp^3 -type orbital.



Scheme 4: Schematic structure of a possible Bi(III) complex with the electron pair in an sp^3 -type orbital.

Based on this observation, I concluded that a Bi(V)–F complex could be a potent electrophilic fluorinating reagent; as a formal F^+ leaves the complex, the fluoride in the parent complex can just be replaced by the electron pair – electrophilic fluorination from a Bi(V) complex could potentially come without significant geometric change in the residual ligand sphere. The rest is ligand design.

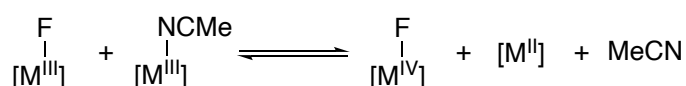
So I came up with a couple of ligand framework structures and tried to modify the electronic properties in a way the Bi(V)–F would be able to fluorinate TEDA without decomposing itself. Unfortunately, I didn't find the sweet spot between reactivity and stability. Nevertheless, here are some structures I looked into:



Scheme 5: Structural backbones of a row of investigated bismuth (III) complexes. The corresponding Bi(V)–F complexes were (unsuccessfully) analyzed regarding their potential to electrophilically fluorinate TEDA.

3.4.3 Back to Group Ten – Ni, Pd, Pt and the Spin Polarization Parameter

Actually, I never really left the group ten fluoride complexes. What eventually brought my focus back to the group 10 fluoride complexes were the reports of the RITTER group regarding an aryl C–F reductive elimination, starting from a M(II) complex with M = Ni, Pd.^{[110],[111]} As it turned out, the reaction with Ni proceeds *via* a Ni(III)–F active intermediate,^[112] while the reaction with Pd proceeds *via* a Pd(IV)–F active intermediate.^[113] In order to understand where this difference comes from, the first thing I analyzed was the Potential Energy Surface (PES) (cf. Fig. 5) of the equilibrium given in scheme 6.



Scheme 6: Schematic equilibrium reaction of M(III)–F and M(IV)–F with M = Ni, Pd, Pt.

While the ΔG_{eq} values reported in fig. 5 are in beautiful agreement with the experimental observations by RITTER *et al.*,^{[110]–[113]} the reason behind this observation is still not clear.

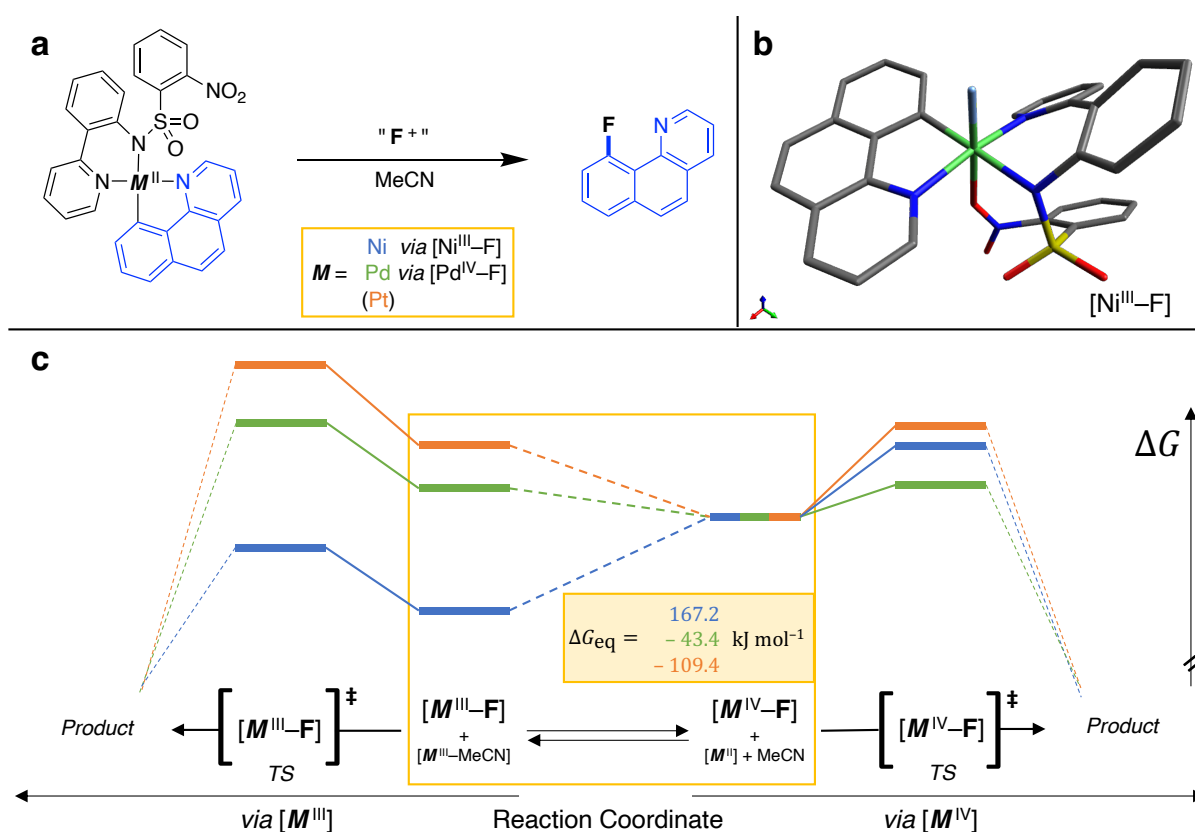


Figure 5: a: Lewis scheme of the investigated reaction by RITTER *et al.* b: Geometry of Ni(III)–F complex as a representative example. c: PES of the equilibrium, including the transition states of the following C–F bond forming reductive elimination reactions, as well as the calculated Free Energies for the displayed equilibrium reaction with M = Ni, Pd, Pt. Method: (CPCM(MeCN) DLPNO-CCSD(T)/DKH2/SARC-DKH-TZVPP/DKH-def2-TZVPP//CPCM(MeCN) PBE0-D3/def2-TZVP).

Here is the current hypothesis: The individual spin orbitals of the doubly occupied orbitals in an open shell system tend to polarize (“split up” energetically). This splitting is highly dependent on the element. As it turns out, the spin orbitals in open shell systems of first row

transition metal systems tend to polarize stronger than those of second or third row transition metals. I am currently trying to parametrize this effect and show that the observed reactivity differences discussed above stem from the differences in these “Spin Polarization Parameters” (SPP).

Why should this spin polarization have such a clear effect on the energetics of the system? When the HOMO of a closed shell system loses one electron, the (now called) SOMO relaxes according to the spin polarizability of the system: the occupied α orbital goes down in energy, while the unoccupied β orbital goes up. As the α orbital is the only one occupied, the overall energy of the system goes down.

What now has to follow is the thorough parametrization of this spin polarizability, and the revelation of the (so far only hypothetical) connection between the resulting parameter and the observed reactivity trend. As this task turns out to be quite complex (and I’m already working on that for the better part of this year), this thesis is completed without the finalization of this project.

One thought, however, I will take out of this project: I have already previously learned that the F-TEDA radical cation is extremely unstable. Maybe the SET/fluoride transfer/SET reaction described above is not the right synthesis mode for F-TEDA, starting from fluoride. Hence, maybe exactly that observed single-electron reactivity of Ni and also Pd (even if less prominent) was the flaw of my approach so far. The proposed solution: move down in the periodic table. The next focus for the electrophilic fluorination of TEDA should maybe lie on Pt and Au – because they might transfer an F^+ without diverging any electron pairs and hence without generating the reactive F-TEDA radical cation intermediate.

4 Summary

The research advances discussed in this thesis include the mechanistic analysis of an aryl C–H fluorination reaction, the theoretical investigation into the electronic difference of oxo and fluoro ligands for transition metals and why there is an oxo (and nitrido) wall, but no fluoro wall, the generation of a segmented all-electron relativistically contracted basis set in triple- ζ quality, and the discussion of the advances on the way to the *umpolung* reaction of fluoride – which is how I call the synthesis of electrophilic fluorinating reagents like F-TEDA from fluoride – including the first introduction of the concept of a “Spin Polarization Parameter”.

In summary, I am extremely happy this giant of a doctoral phase finally comes to an end. I hope the research advances described in this thesis help us as a scientific community to come closer to the objective of my research in the last half decade, said *umpolung* reaction of fluoride. Especially those thoughts described in the last subchapter are still full of potential – at least in my eyes. I will certainly not stop digging into these thoughts, as much as I hope they might also inspire others to do the same.

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Eidesstattliche Erklärung

Hiermit erkläre ich, Julian David Rolfes, an Eides Statt, dass ich die vorliegende Arbeit mit dem Titel

„About chemical Trends in Transition Metal Complexes“

selbstständig und ohne Benutzung anderer als der angegebenen Quellen und Hilfsmittel sowie fremder Hilfe angefertigt habe.

Alle Stellen, die wörtlich oder sinngemäß aus veröffentlichten oder nicht veröffentlichten Schriften entnommen wurden, sind als solche kenntlich gemacht. Die Arbeit hat in gleicher oder ähnlicher Form noch keiner Prüfungsbehörde vorgelegen.

Zu den dieser Arbeit zugrundeliegenden Publikationen habe ich folgende Beiträge geleistet:

- „Palladium–catalysed electrophilic aromatic C–H fluorination“^[2]: Vollständige computerchemische Evaluation; Mitarbeit an mechanistischen Studien, Substrat-Scope, Datenanalyse.
- „Where Is the Fluoro Wall?: A Quantum Chemical Investigation“^[3]: Vollständige computerchemische Evaluation sowie Verfassen des Manuskriptes.
- „All-Electron Scalar Relativistic Basis Sets for the Elements Rb–Xe“^[4]: Vollständige Entwicklung des Basissatzes; Mitarbeit an der Evaluation der Qualität sowie Verfassen des Manuskriptes.

(Ort, Datum)

(Unterschrift)

A Appendix

Appended are all academic – or rather: topic-related (peer-reviewed) and other (not necessarily peer-reviewed) publications I worked on during the time of my doctoral studies at the MAX-PLANCK-INSTITUT FÜR KOHLENFORSCHUNG from 2016 to 2020.

A1 – Academic Publications

A1.1 “Palladium–catalysed electrophilic aromatic C–H fluorination”^[2]

A1.2 “Where Is the Fluoro Wall?: A Quantum Chemical Investigation”^[3]

A1.3 “All-electron scalar relativistic basis sets for the elements Rb–Xe”^[4]

A2 – Other Publications

A2.1 “Making Science Organizations Sustainable – The Mission of the Max Planck Sustainability Network”^[114]

A2.2 “The “Me too” movement from Hollywood to your bench”^[115]

A2.3 “Voluntary Commitment: Climate-Friendly Business Trips – An Overnight Miracle”^[116]

A2.4 “Should I stay or should I go (out)?”^[117]

A2.5 “Black Lives Matter – Black Minds Matter”^[118]

A2.6 “Nachhaltigkeits-Netzwerk der Max-Planck-Gesellschaft – Interimsstatuten / Max Planck Sustainability Network – Interim Statutes”

A2.7 “Max-Planck-Nachhaltigkeits-Netzwerk – Statuten / Max Planck Sustainability Network – Statutes”

A2.8 An open letter to the Max Planck Society – appeal for nonbinary inclusive language. (English original + German translation incl. authors’ comment)

A2.9 “Aufruf zur Selbstverpflichtung der Mitarbeitenden der Max-Planck-Gesellschaft: Klimafreundliche Dienstreisen / Call for Voluntary Commitment by the Coworkers of the Max Planck Society: Climate-Friendly Business Trips”

A2.10 “Kompensation von CO₂-Emissionen durch Reiseaktivitäten in der Max-Planck-Gesellschaft”

A2.11 “Kritischer Kommentar zum vorliegenden Fachbeitrag „Fachbeitrag Wasserrahmenrichtlinie für den Neubau der A 49 im Abschnitt Stadtlendorf – Gemünden (VKE 40)“ von der ahu GmbH vom 28.09.2020.”

A1.1 “Palladium–catalysed electrophilic aromatic C–H fluorination”^[2]

Palladium-catalysed electrophilic aromatic C–H fluorination

Kumiko Yamamoto^{1,2*}, Jiakun Li^{1*}, Jeffrey A. O. Garber^{1,2}, Julian D. Rolfes^{1,2}, Gregory B. Boursalian^{1,2}, Jannik C. Borghs², Christophe Genicot³, Jérôme Jacq³, Maurice van Gastel¹, Frank Neese¹ & Tobias Ritter^{1,2}

Aryl fluorides are widely used in the pharmaceutical and agrochemical industries^{1,2}, and recent advances have enabled their synthesis through the conversion of various functional groups. However, there is a lack of general methods for direct aromatic carbon–hydrogen (C–H) fluorination³. Conventional methods require the use of either strong fluorinating reagents, which are often unselective and difficult to handle, such as elemental fluorine, or less reactive reagents that attack only the most activated arenes, which reduces the substrate scope. A method for the direct fluorination of aromatic C–H bonds could facilitate access to fluorinated derivatives of functional molecules that would otherwise be difficult to produce. For example, drug candidates with improved properties, such as increased metabolic stability or better blood–brain-barrier penetration, may become available. Here we describe an approach to catalysis and the resulting development of an undirected, palladium-catalysed method for aromatic C–H fluorination using mild electrophilic fluorinating reagents. The reaction involves a mode of catalysis that is unusual in aromatic C–H functionalization because no organometallic intermediate is formed; instead, a reactive transition-metal-fluoride electrophile is generated catalytically for the fluorination of arenes that do not otherwise react with mild fluorinating reagents. The scope and functional-group tolerance of this reaction could provide access to functional fluorinated molecules in pharmaceutical and agrochemical development that would otherwise not be readily accessible.

Conventional methods for aromatic fluorination require elemental fluorine or similarly reactive reagents, which are unselective and require specialized equipment to handle safely⁴. Bench-stable electrophilic fluorinating reagents—such as *N*-fluoropyridinium salts, *N*-fluorobenzenesulfonimide (NFSI) and Selectfluor—are easier to handle but less reactive, and require either very electron-rich arenes or multiple equivalents of the arene to accomplish direct C–H fluorination^{5,6}. Catalysis of aromatic C–H fluorination reactions has been reported using coordination-assistance to promote fluorination proximal to Lewis-basic functional groups, but such approaches are limited in scope to those substrates containing the required directing groups^{7–10}. Advances in aliphatic C–H fluorination have been made¹¹, but currently there is no method for direct aromatic C–H fluorination with broad scope.

In our investigation into the catalysis of aromatic C–H fluorination reactions, we sought an approach that was distinct from the common C–H activation sequence in which C–H metalation precedes functionalization; with few exceptions^{12–14}, the conventional approach¹⁵ requires multiple equivalents of the arene substrate to promote C–H metalation in the absence of a coordinating directing group. Instead, we sought to design catalysts with ancillary ligands that would favour the oxidation of the complex before any interaction with the substrate, giving rise to a reactive, high-valent metal–fluoride intermediate that

is electrophilic at fluorine and capable of oxidative fluorine transfer to arenes. We designed the Pd(II) complex **1**, ligated simultaneously by a tridentate (terpyridine, terpy) and a bidentate (2-chloro-1,10-phenanthroline, 2-Cl-phen) ligand, which would be oxidized by electrophilic fluorinating reagents to yield the desired Pd(IV)–F complex **2** (Fig. 1b). The oxidation of doubly cationic **1** is promoted by a destabilizing interaction between the lone pair of the apical donor atom and the filled d_{z^2} orbital on Pd(II), which is readily apparent in the highest occupied molecular orbital of **1** as calculated by density functional theory (DFT) (Fig. 1c). X-ray diffraction corroborates the apical interaction: the

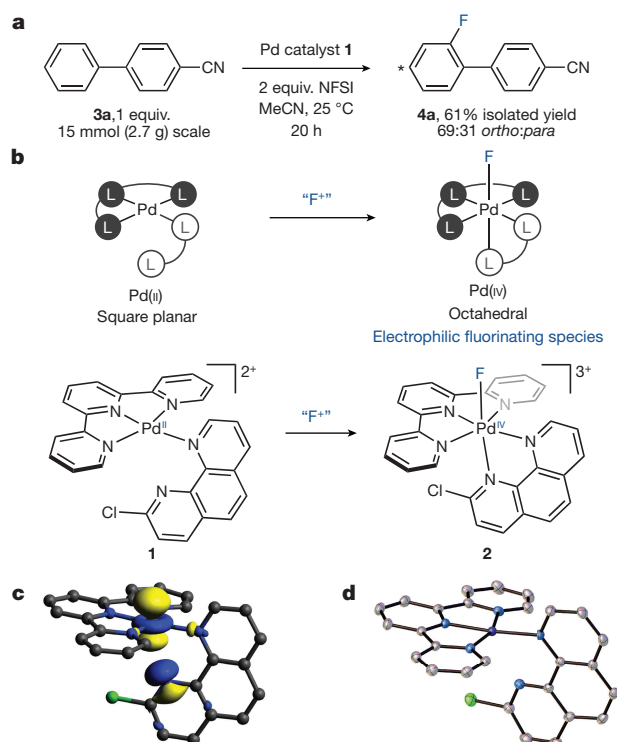


Figure 1 | Aromatic fluorination catalysed by 1. **a**, Palladium catalyst **1** enables the direct, non-chelation-assisted fluorination of 4-cyanobiphenyl. **b**, Oxidation of Pd(II) complex **1**, assisted by the ligand combination of terpy and 2-Cl-phen, yields the triply cationic Pd(IV)–F electrophile **2**. **c**, The highest occupied molecular orbital of **1**, as calculated by DFT, showing destabilizing orbital interaction. Hydrogen atoms are omitted for clarity. Calculations at the CPCM(MeCN)TPSS0 D3/def2-QZVP//PBE0 D3/def2-TZVP level of theory; iso = 0.05. **d**, X-ray crystal structure of **1**, shown with 50%-probability ellipsoids. Hydrogen atoms and solvent molecules are omitted for clarity.

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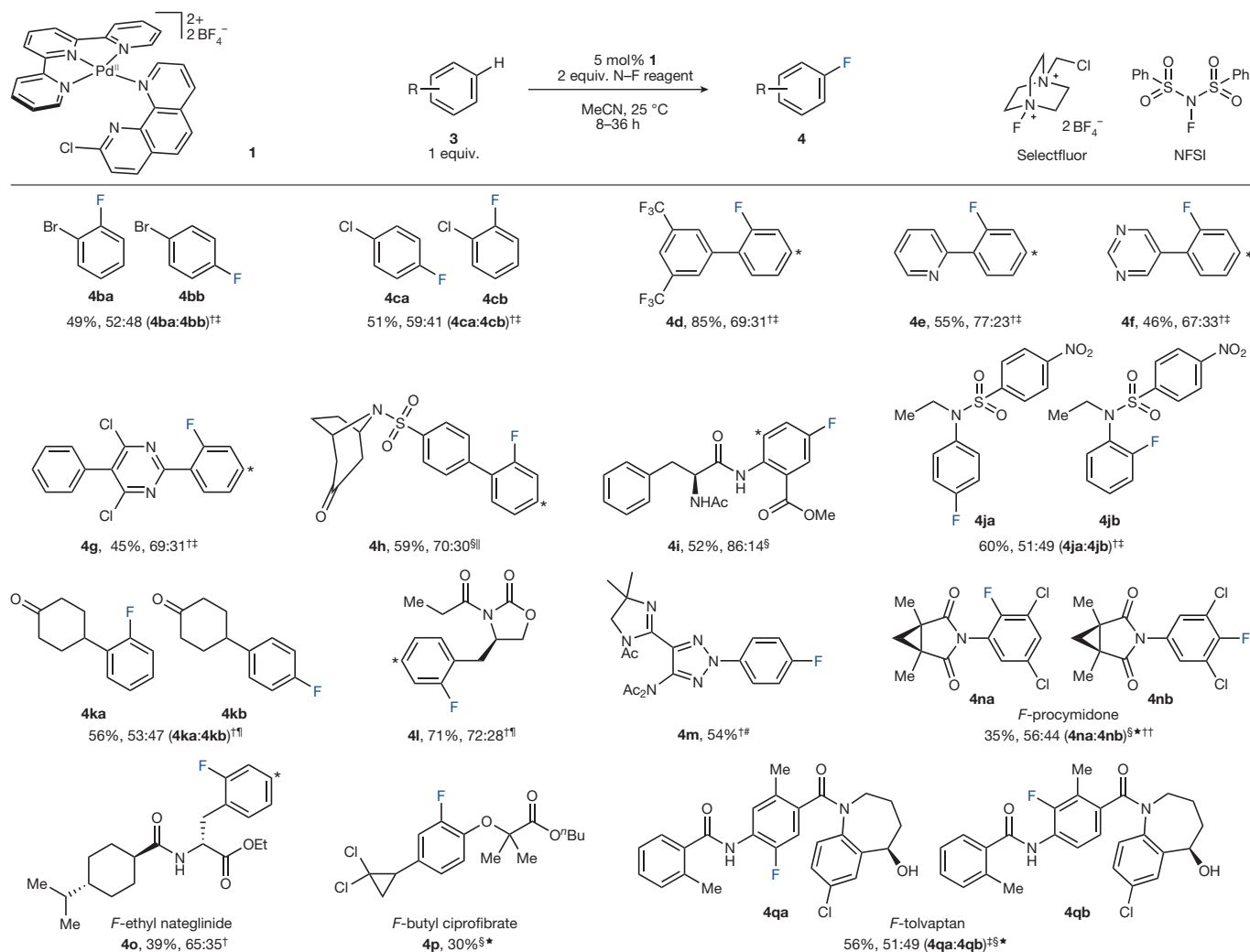


Figure 2 | Substrate scope of the Pd-catalysed fluorination of arenes.

Reaction conditions: arene, 1 mmol; catalyst **1**, 5 mol%; Selectfluor or NFSI, 2 equiv.; MeCN, 0.1 M. All isomers of non-volatile products have been isolated and characterized as analytically pure samples. The asterisk denotes the site of fluorination of the constitutional isomer that is not shown. Overall yields and the ratio of the constitutional isomers

Pd–N distance in the X-ray structure of **1** (Fig. 1d) is 2.6 Å, which is 1.2 Å shorter than the sum of the van der Waals radii of Pd and N (ref. 16).

Complex **1** is a competent catalyst for the fluorination of various arenes by either Selectfluor or NFSI. The substrates shown in Fig. 2 underwent fluorination in the presence of **1** at room temperature or at 50 °C, but little background reactivity was observed in the absence of **1** under otherwise identical conditions (maximum <1% yield) or even under reflux in acetonitrile (maximum 21% yield). In our studies, catalyst **1** was formed *in situ* from [Pd(terpy)(MeCN)](BF₄)₂ and 2-Cl-phen, but it can also be generated by combining the commercially available palladium source [Pd(MeCN)₄](BF₄)₂ and the ligands before the addition of the reactants. Compatible functional groups include nitriles (**3a**), aryl bromides (**3b**), chlorides (**3c**, **3g**, **3n**, **3p**, **3q**), certain heterocycles (**3e–3g**, **3m**), sulfonamides (**3h**, **3j**), ketones (**3h**, **3k**), amides (**3i**, **3l–3o**, **3q**), esters (**3i**, **3o**, **3p**), carbamates (**3l**), ethers (**3p**) and free hydroxy groups (**3q**). Five-membered heteroarenes containing nitrogen (**3m**) can be tolerated, but oxidatively labile functional groups such as amines and thiols cannot, owing to their general incompatibility with electrophilic fluorinating reagents. Electron-deficient arenes such as **3b–3d** are not successfully fluorinated through conventional methodologies, but are suitable substrates for fluorination via catalysis with **1**. However, more electron-deficient arenes, such as methyl benzoate, are insufficiently reactive and undergo little or no conversion.

are based on ¹⁹F NMR integration of reaction mixtures with internal standard. †Reaction performed with Selectfluor. ‡Reaction performed at 50 °C. §Reaction performed with NFSI. ||Reaction performed with 1,2-dichloroethane and MeCN (1:1, 0.1 M). ¶Reaction performed at 0 °C. #10 mol% catalyst **1** was used. *7.5 mol% catalyst **1** was used. ††Reaction performed at 80 °C.

Structurally complex substrates—such the pesticide procymidone (**3n**), the type-2 diabetes drug nateglinide (**3o**), the lipid-lowering agent ciprofibrate (**3p**) and the hyponatremia drug tolvaptan (**3q**)—were fluorinated directly via catalysis with **1**. Although fluorine can impart desirable properties on pharmaceuticals and agrochemicals, fluorinated analogues of structurally complex molecules can currently be difficult to access; conventional fluorination methods failed to provide the fluorinated products shown in Fig. 2.

In most cases, the fluorination reaction affords mixtures of at least two constitutional isomers, resulting from similar rates of fluorination at the positions *ortho* and *para* to the aromatic substituents. Purification of aryl fluoride products from mixtures of their constitutional isomers and the starting material is often challenging^{17,18}. However, the isolation and characterization of all the non-volatile products obtained here has been achieved, although optimization of the separation protocol was required for each substrate. For example, the *ortho*- and *para*-fluorinated products of the gram-scale fluorination of 4-cyanobiphenyl have been separated in 61% isolated yield (Fig. 1a). Although high positional selectivity is generally desired in C–H functionalization reactions, mixtures of constitutional isomers can be advantageous for some applications. For example, in the late-stage derivatization of drug candidates, each product isomer is an additional derivative that can be obtained without the need for costly and laborious *de novo* synthesis^{19,20}. Fluorinated tolvaptan

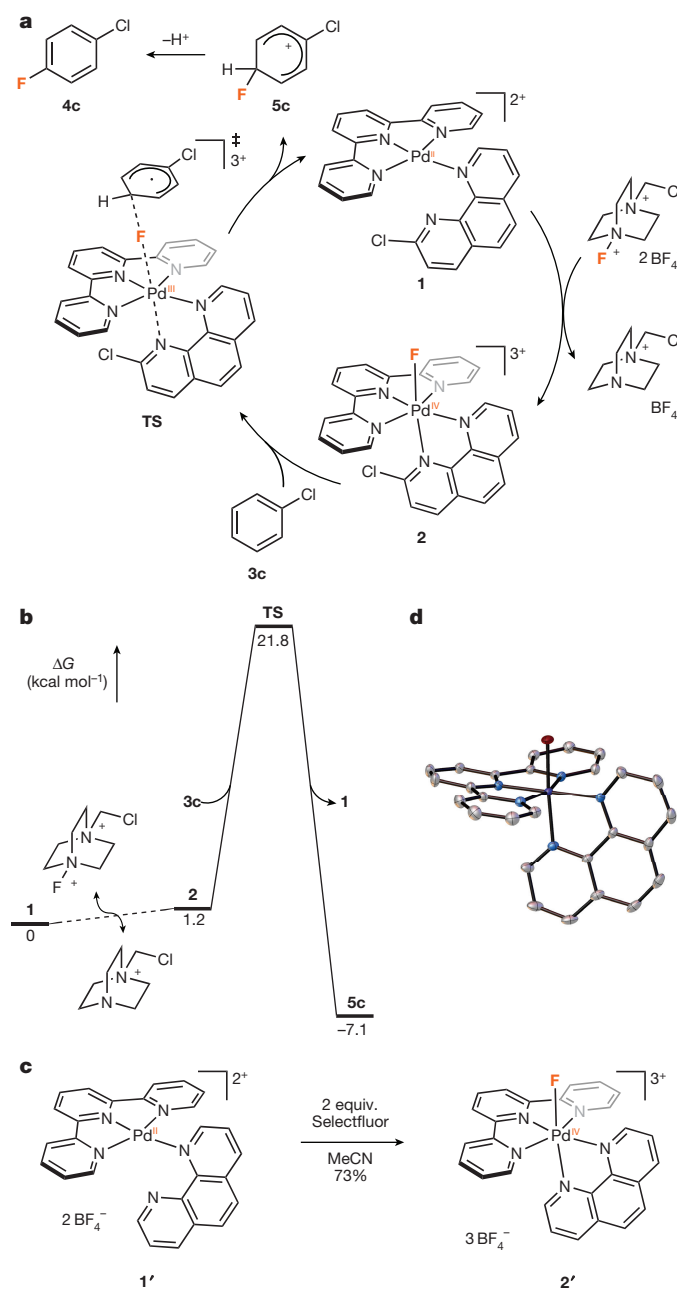


Figure 3 | Mechanism of fluorination catalysed by 1. **a**, The proposed catalytic cycle for the fluorination of chlorobenzene (3c). **b**, Energy-level diagram of the proposed catalytic cycle with chlorobenzene (3c); energies calculated by DFT. **c**, Synthesis of Pd(IV)-F complex **2'** via the oxidation of **1'** by Selectfluor. **d**, X-ray crystal structure of **2'**, shown with 50%-probability ellipsoids. Pd-F bond length: measured, 1.9120(7) Å; calculated, 1.89 Å.

(4q), for example, would be challenging and time-consuming to prepare with conventional chemistry through *de novo* syntheses. Late-stage fluorination, even with the requirement for a custom-made separation protocol, can conveniently produce promising new candidates that may have never been evaluated otherwise.

The proposed mode of action of **1** is highly unusual in the catalysis of aromatic oxidation reactions: conceptually, an activated electrophile is generated *in situ* from **1**, in the form of Pd(IV)-F intermediate **2**. The activated Pd(IV)-F electrophile **2** would therefore be capable of electrophilic fluorination of weakly nucleophilic arenes that cannot be fluorinated directly by Selectfluor and NFSI (Fig. 3a)^{21,22}. A DFT analysis of the aryl fluorination reaction suggests a mechanism that is accessible to Pd(IV)-F **2** but not to Selectfluor or NFSI. On the basis of these results,

we hypothesize that the fluorination mechanism proceeds through a single transition state via fluoride-coupled electron transfer (Fig. 3a, b).

Selectfluor fluorinates only electron-rich arenes such as anisole²³; complex **1**, conversely, is able to catalyse the fluorination of electron-deficient arenes such as chlorobenzene. DFT calculations suggest that Pd(IV)-F **2** has a higher single-electron reduction potential than that of Selectfluor, although both compounds have a similar thermodynamic driving force for electrophilic fluorination. The transition state TS of the fluorination of chlorobenzene with Pd(IV)-F **2** shows high spin-density on the Pd as well as on the aryl carbon atoms. As such, the transition state is most appropriately characterized as a singlet diradical; two subsequent fluoride-coupled electron transfers occur asynchronously as the reaction proceeds through a single transition state. The mechanism is reminiscent of that previously reported for the fluorination of enamines and organometallic reagents with an isolated Pd(IV)-F (ref. 24). The calculated energy barrier for electrophilic fluorination of 21.8 kcal mol⁻¹ (Fig. 3b) is in agreement with the observed reaction time and the temperature of the reaction (as discussed below, see Supplementary Information for details).

We sought to produce Pd(IV)-F complex **2**, to verify our design principle as well as to investigate the reactivity of **2** with arenes. Treatment of **1** with XeF₂ in the presence of LiBF₄ produced a ¹⁹F NMR signal attributable to **2** at $\delta = -258.6$ p.p.m.; however, complex **2** is reduced to **1** in acetonitrile solution, even in the absence of substrate, which hindered our attempts at isolation. Treatment of **1** with Selectfluor over a range of temperatures (-40 °C to 25 °C) resulted in the desired reduction of Selectfluor, but did not produce a ¹⁹F NMR signal that could be attributed to a Pd(IV)-F species, presumably because **2** is reduced faster than it is formed under these conditions, and therefore does not accumulate in observable quantities.

Complex **1'**, in which 2-Cl-phen is replaced with unsubstituted phenanthroline (phen), is a competent catalyst for aromatic fluorination, although not as effective as catalyst **1**. When **1'** was treated with Selectfluor in acetonitrile at room temperature and then allowed to stand at -35 °C, the Pd(IV)-F complex **2'** (¹⁹F NMR -259.5 p.p.m.) precipitated in 73% yield (Fig. 3c). Complex **2'** is sufficiently stable at low temperature to enable characterization and reactivity studies. The higher stability of **2'** as compared to **2** is understood to result from the greater electron-donating ability of phen relative to that of 2-Cl-phen. Likewise, the greater reactivity of **2** may explain why the 2-Cl-phen-ligated complex **1** outperforms the phen-ligated **1'** in terms of catalytic ability.

Pd(IV)-F complex **2'** reacts with arenes to yield fluorinated products (Fig. 4). For example, 4-cyanobiphenyl (**3a**), when treated with **2'** in acetonitrile, yielded a 66:34 ratio of *ortho*- and *para*-fluoro isomers in 63% overall yield. The positional selectivity of fluorination by **2'** is similar to that observed in fluorination catalysed by **1'** (69:31 *ortho:para*), consistent with **2'** being the C-F bond-forming species in catalysis by **1'**. These selectivity ratios are, in turn, similar to that observed upon fluorination with the optimal 2-Cl-phen-ligated catalyst **1** (71:29 *ortho:para*). We cannot rule out the involvement of a different C-F bond-forming pathway in catalysis by **1** (for example, through a Pd(III) species); however, the similar positional selectivities observed in fluorination catalysed by **1**, fluorination catalysed by **1'**, and stoichiometric fluorination by **2'** are consistent with fluorination by similar Pd(IV)-F species in all three cases, corresponding to **2** in the case of catalysis by **1**.

Aromatic C-H oxidations catalysed by transition metals generally proceed via C-H metalation followed by oxidation of the resulting organometallic intermediate, with product formation ensuing through reductive elimination. The aromatic fluorination catalysed by **1** presented here is an unusual example of an alternative mode of catalysis for aromatic C-H oxidation, in which a transition-metal catalyst is oxidized to a high-valent intermediate, which in turn oxidizes the substrate by group transfer of a ligand. Such an 'oxidation-first' mechanism is reminiscent of various transition-metal-catalysed aliphatic C-H oxidations, such as hydroxylations²⁵⁻²⁷ and halogenations²⁸ through high-valent metal-oxo complexes, and aminations²⁹ via metal-nitrenoid

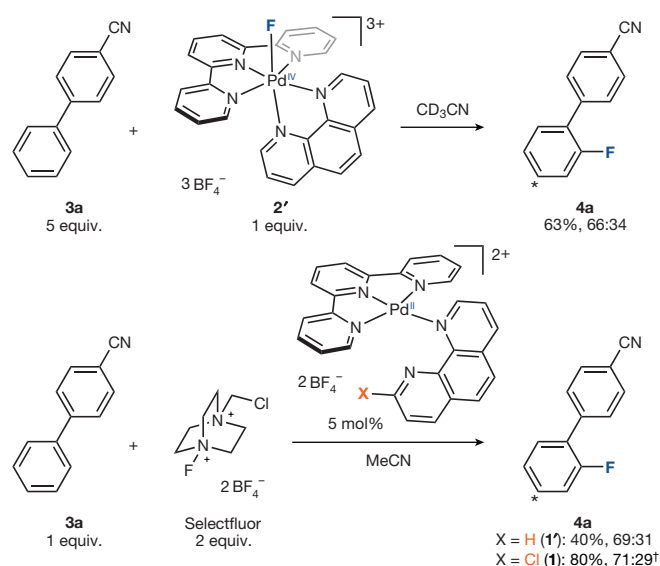


Figure 4 | Comparison of the positional selectivity of stoichiometric and catalytic fluorinations using 2'. Top, stoichiometric fluorination; bottom, catalytic fluorination. †5 equiv. of 4-cyanobiphenyl (3a) and 1 equiv. of Selectfluor were used.

species. Reported examples of such a mechanism for aromatic C–H oxidation, however, are rare, and are proposed to involve metal-nitrene or aminyl-radical transfer to the arene, although evidence for the proposed modes of action in these cases is indirect^{30,31}. To the best of our knowledge, the aromatic fluorination reaction reported here is the only example so far of a synthetic method for aromatic C–H functionalization in which oxidation reactivity between a high-valent catalytic intermediate and arenes has been directly scrutinized.

The other examples of aromatic and aliphatic C–H oxidation reactions proceeding through ‘oxidation-first’ mechanisms mentioned above function because the high-valent intermediate provides access to a mechanism of oxidation that is not available to the starting reagents, such as a radical-rebound mechanism in the case of hydroxylation through metal–oxo intermediates. We have shown here data that support the interpretation that catalyst **2** provides access to a fluoride-coupled electron-transfer mechanism that is not accessible to electrophilic fluorinating reagents such as Selectfluor.

We anticipate that the direct electrophilic C–H fluorination of arenes reported here will be a useful tool in medicinal chemistry; indeed, the reaction has already found use in the late-stage derivatization of drug molecules. Furthermore, the unusual mechanism of catalysis by complex **1**, in which a high-valent transition-metal intermediate undergoes group transfer to arenes, may become the basis for a new approach to the catalysis of C–H functionalization reactions.

Data Availability Data are available from the corresponding author on reasonable request.

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Supplementary Information is available in the online version of the paper.

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Author Contributions K.Y. designed catalyst **1** and optimized the fluorination reaction. K.Y. and J.D.R. conducted mechanistic studies. K.Y. and G.B.B. developed the conceptual approach to the project. J.L., J.A.O.G., J.C.B., K.Y. and J.D.R. explored the substrate scope. J.D.R. performed DFT calculations with input from M.v.G. and F.N. G.B.B. wrote the manuscript with input from all other authors. C.G. and J.J. supported development towards useful examples. K.Y., J.L., J.A.O.G., G.B.B., J.D.R. and T.R. analysed the data. T.R. directed the project.

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A1.2 “Where Is the Fluoro Wall?: A Quantum Chemical Investigation”^[3]

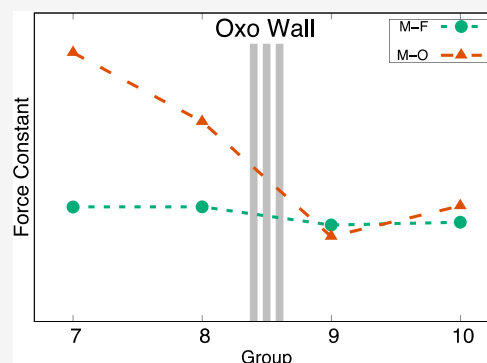
Where Is the Fluoro Wall?: A Quantum Chemical Investigation

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S Supporting Information

ABSTRACT: Despite their isoelectronic properties, fluoro and oxo ligands exhibit completely different chemical behavior. Formally speaking, the first is known to exclusively form single bonds, while the latter is generally observed to form double (or even triple) bonds. The biggest difference, however, lies in what is known among inorganic chemists as the Oxo Wall: the fact that six-coordinate tetragonal transition metal oxo complexes are not observed beyond group 7 elements. While the Oxo Wall was explained a few decades ago, some questions regarding the nature of the Oxo Wall remain unanswered. For example, why do group 8 oxo complexes with high oxidation states not violate the Oxo Wall? Moreover, why are transition metal fluoro complexes observed through the whole transition metal series? In order to understand how the small difference between these two isoelectronic ligands can give rise to such different chemical behaviors, we conducted an extensive computational analysis of the geometric and electronic properties of model fluoro and oxo complexes with metals around the Oxo Wall. Among many insights into the details of the Oxo Wall, we mostly learned that the oxygen 2p orbitals are prone to meaningfully interact with transition metal d orbitals, because they match not only spatially but also energetically, while for fluorine the p orbital energies are lower to an extent that interaction with transition metal d orbitals is much reduced. This in turn implies that in those instances where the metal d orbitals principally accessible for interaction are occupied, the oxygen 2p orbitals are too exposed to be stable.



INTRODUCTION

The Oxo Wall is a widely known and accepted concept among the inorganic chemical community.¹ It states the instability of six-coordinate tetragonal oxo complexes with metals beyond group 8 (Figure 1).

7	8	9	10
²⁵ Mn	²⁶ Fe	²⁷ Co	²⁸ Ni
⁴³ Tc	⁴⁴ Ru	⁴⁵ Rh	⁴⁶ Pd
⁷⁵ Re	⁷⁶ Os	⁷⁷ Ir	⁷⁸ Pt

Figure 1. Depiction of the Oxo Wall surrounded by the investigated transition metals.

While transition metal oxo complexes are a prominent motif in biological oxidation processes,^{2,3} the concept of the Oxo Wall dates back to 1962 when Ballhausen and Gray developed a molecular orbital energy level scheme that correctly described the electronic structure of the vanadyl ion.⁴ The description of chromyl and molybdenyl ions followed shortly after, where the metal–oxo interaction was represented as a triple bond for the first time.⁵ This notion is based on elementary molecular orbital considerations in which the bond

order is deduced by subtracting the number of electrons in antibonding orbitals of a given bond from the number of electrons in the bonding counterparts of these orbitals and dividing the result by two.⁶ For example, in the six-coordinate tetragonal oxo complex Mo(V)OCl_5^{2-} the single d electron is found in the nonbonding d_{xy} orbital, leaving the two other d orbitals of t_{2g} symmetry (d_{xz} and d_{yz}) amenable to π interactions with the $p_{x/y}$ orbitals from the oxo ligand on the z axis (Figure 2). A total of six electrons are present in the two bonding π -orbitals and the bonding σ -orbital (interaction between oxo p_z and metal d_z^2 orbital), while all antibonding counterparts are empty, thus leaving a metal–oxo triple bond.

The theoretical concept of the Oxo Wall—as stated by Gray and Winkler—is as follows: “Complexes with tetragonal symmetry can have no more than 5 d electrons and still retain some MO multiple bonding. In the absence of π -bonding to the metal, the oxo will be extremely basic and unstable with respect to protonation or attack by electrophiles.”¹ This is also supported by a large array of experimental investigations.^{7–9} While oxo compounds are known with transition metals beyond the Oxo Wall^{10,11} with well-characterized electronic structure,¹² these do not violate the concept of the Oxo Wall because they are not of tetragonal symmetry. Claims that exceptions have been found¹³ were later retracted and as such, “the ‘Oxo Wall’ stands.”¹⁴

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RESULTS

Geometries. The M–X bond lengths of the most stable spin states (ground states) of the calculated complexes are summarized in Table 1. In addition, a N–M–N bond angle is

Table 1. Group and Formal Metal d Electron Count, M–X Bond Lengths, (py)N–M–N(py) Bond Angles (along y Axis), and Ground-State Spin Multiplicities ($2S + 1$) for All Calculated M–X Complexes

group	metal center	X = F			X = O		
		M–F bond length [Å]	N–M–N angle [deg]	spin mult.	M–O bond length [Å]	N–M–N angle [deg]	spin mult.
7 (d^3)	Mn	1.769	176.1	4	1.655	166.5	4
	Tc	1.879	166.5	4	1.687	151.1	2
	Re	1.904	164.9	4	1.707	148.5	2
8 (d^4)	Fe	1.741	177.1	3	1.629	168.1	3
	Ru	1.848	167.5	3	1.753	162.1	3
	Os	1.874	166.0	3	1.782	159.7	3
9 (d^5)	Co	1.773	179.5	2	1.790	176.1	2
	Rh	1.905	176.7	2	1.892	171.6	2
	Ir	1.900	171.7	2	1.887	171.4	2
10 (d^6)	Ni	1.789	179.6	1	1.792	175.3	3
	Pd	1.923	179.3	1	1.899	177.8	1
	Pt	1.946	179.5	1	1.921	178.9	1

given that refers to the pyridyl moieties on the y-axis. This angle is a reasonable measure for the deviation from six-coordinate tetragonal geometry, which is especially important for group 9 and 10 complexes (those beyond the Oxo Wall). The full spin-state analysis as well as the ground-state complex geometry coordinates are given in the Supporting Information.

Force Constants. While bond lengths are known to be a reasonable indicator of bond strength, other geometric parameters like bond angles influence the M–X bond length and prevent a clear-cut correlation between the bond length and bond strength. Therefore, the M–X force constants were analyzed, because they provide a more direct and reliable measure of the bond strength (Figure 4). The force constants of the M–F bonds only show minor variations (2.7–4.2 mdyn/Å). The force constants of the M–O bonds, however, reveal a greater variance (1.9–7.9 mdyn/Å) with a clear and consistent discontinuity between group 8 and 9 elements, exactly at the location of the Oxo Wall.

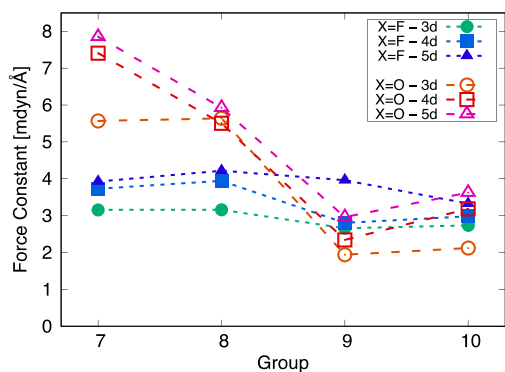


Figure 4. Force constants of M–X bonds for X = F and X = O. Exact values are given in the Supporting Information.

The force constants in Figure 4 indicate that the oxo ligand tends to form bonds of higher order for group 7 and 8 complexes whereas the fluoro ligand does not—which is in agreement with Lewis structure considerations and experimental observations,⁴¹ and also with theoretical studies of transition metal fluoro complexes.^{42,43} In order to understand the origin of this behavior, as well as the weak bonding of the oxo ligand with group 9 elements, the orbital structure of the complexes was analyzed.

Electronic Structure. Orbital Pattern. As a representative picture for all complexes, the 3d quasi-restricted orbitals (QRO) of the Mn–F and Mn–O complexes are presented in Figure 5.

As expected, the d-orbitals in the six-coordinate tetragonal complexes are separated into a low-lying t_{2g} -like set and a higher-lying e_g -like set, in accordance with approximate O_h symmetry. The lowest orbital is the nonbonding d_{xy} orbital. The large separation of the t_{2g} and e_g sets explains why most of the d^3 systems (Mn, Tc, Re) as exemplified in Figure 5 have a $S = 3/2$ ground state, why the d^4 systems (Fe, Ru, Os) are $S = 1$, why the d^5 systems (Co, Rh, Ir) are $S = 1/2$, and why most of the d^6 systems (Ni, Pd, Pt) are $S = 0$ (cf. Table 1). There are two exceptions to these general observations. The first is the low-spin configuration for the d^3 complexes Tc–O and Re–O ($S = 1/2$), which upon inspection of the orbital structure of these complexes is a consequence of the increased energy difference between the lowest nonbonding t_{2g} orbital and the two antibonding π^* type t_{2g} orbitals (intra- t_{2g} splitting). For Tc–O and Re–O, this energy gap is large enough that the double population of the lowest orbital is energetically favorable, leaving the highest t_{2g} orbital empty. The second is the Ni–O complex (d^6), which features a triplet ground state with a singly occupied orbital from the e_g set (*vide supra*). The localization and stabilization of the lowest e_g orbital indicates that the weakest ligand field is induced by the aliphatic nitrogen atoms of the ligand. We will come back to this subject later in the framework of the angular overlap model.

A thorough comparative analysis of the composition of the QROs of the fluoro and oxo complexes led to two interesting observations. Most noticeably, the oxo complexes of the group 9 elements as well as the Ni–O complex hold a singly occupied p orbital rather localized on the oxo ligand than on the metal (cf. Figure 6), even though this orbital formally constitutes the energetically highest orbital of the t_{2g} set. The presence of a singly occupied p(O) orbital implies a formal metal oxidation state of III instead of the expected oxidation state of IV, rendering the oxo ligand as an oxyl radical ligand. While one would intuitively expect the singly occupied orbital of the group 9 elements to be a metal d orbital, the large p(O) character of the e_g orbital indicates that the order of the d(M) and p(O) orbitals has changed and that from group 9 on, the p(O) orbitals are the highest (singly) occupied QROs. The formal oxidation state of III implies a d electron count of 6 instead of 5 for the group 9 elements, all located in the t_{2g} orbitals set. In other words, one could say that the p(O) orbitals can no longer sufficiently interact with the d(M) orbitals, resulting in a formal bond order of 1. Together with the reduced oxidation state of the metal and the transformation of the oxo ligand into a weaker bonding oxyl radical ligand, the significant and uniform reduction of the force constant for the group 9 M–O complexes (cf. Figure 4) is a logical consequence.

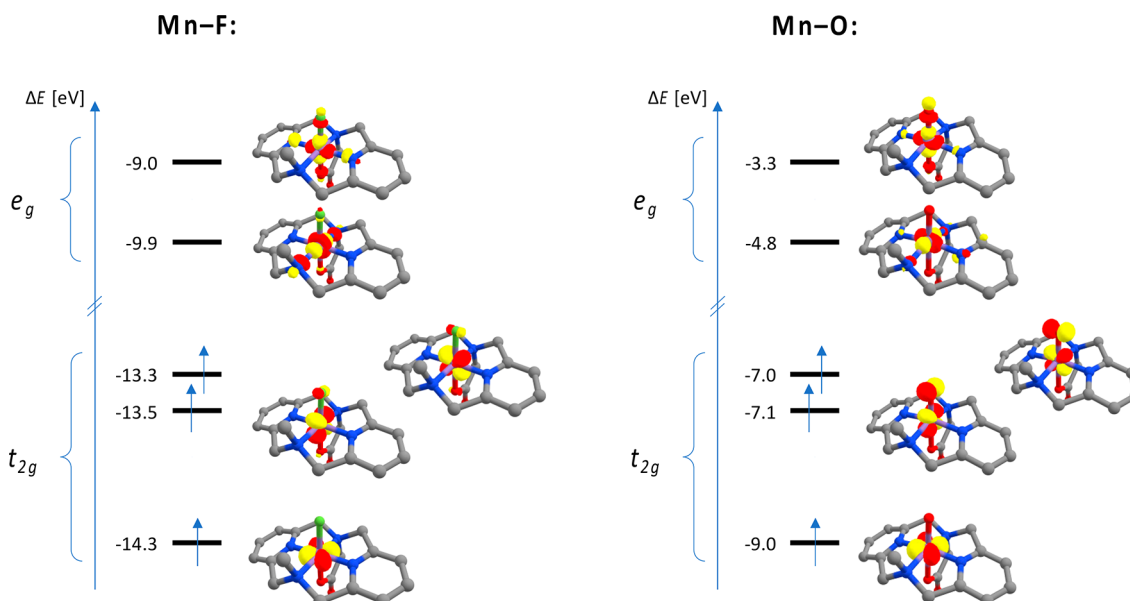


Figure 5. Representative orbital diagram for the d type QROs with energies, orbital pictures, and grouping terms (t_{2g} , e_g ; note that these are descriptive terms only and do not state actual degeneracy) of Mn–F (left) and Mn–O (right) complexes. Hydrogens are omitted for clarity (PBE0-D3/def2-TZVP, iso = 0.1).

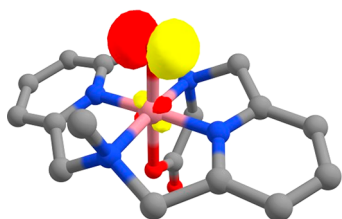


Figure 6. Singly occupied QRO of the Co–O complex. Hydrogens are omitted for clarity (PBE0-D3/def2-TZVP, iso = 0.1).

The latter analysis also holds true for the Ni–O complex, which is the only group 10 complex with a triplet ground state. The QROs reveal a singly occupied p(O) orbital as well as a singly occupied orbital that can be described as a $d_{x^2}(\text{Ni})$

orbital. These two orthogonal orbitals are close enough in energy to give rise to a high-spin configuration, resulting in a Ni(III) center with an oxyl radical ligand. Figure 7 gives a comprehensive overview of the electronic ground states of the calculated group 9 and 10 oxo and fluoro complexes. The increased d electron count in the Ni–O complex results in a bond length extension of all nickel–ligand bonds, most noticeably for the aliphatic amines, which are the weakest ligands. The force constant of the Ni–O bond, of a value in between those of the Co–O and the Rh–O bonds, is also in agreement with this interpretation (cf. Figure 4).

The elevated radical character on oxygen in the formal $\text{Co}^{\text{III}}\text{--O}$, $\text{Rh}^{\text{III}}\text{--O}$, and $\text{Ir}^{\text{III}}\text{--O}$ complexes directly to the right side of the Oxo Wall (Figure 1) and that of the $\text{Ni}^{\text{III}}\text{--O}$ complex explains why it has so far proven elusive to synthesize

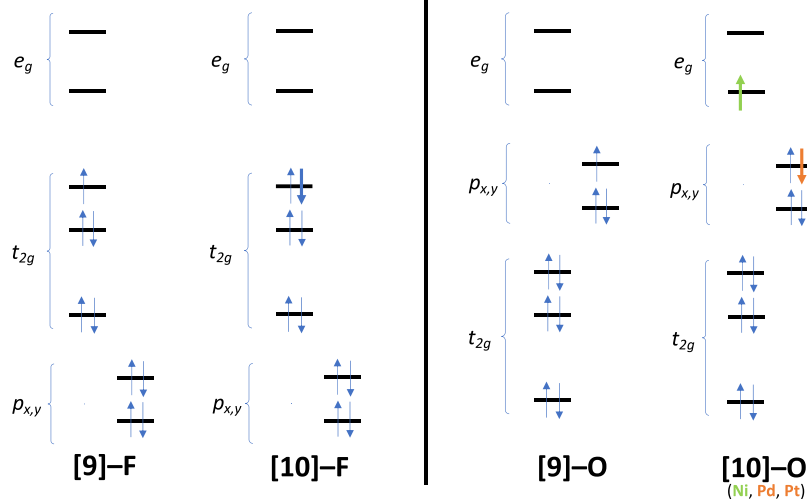


Figure 7. Qualitative depiction of the group 9 ([9]) and 10 ([10]) complexes' electronic ground states. The difference for the group 10 oxo complexes is shown through color: The green electron in the e_g orbital depicts the high-spin ground state of the Ni–O complex, while the orange electron in the p orbital depicts the low-spin ground state of the Pd–O and Pt–O complexes.

such compounds. Even though the basic theoretical explanation of the Oxo Wall concept in principle allows for the existence of six-coordinate tetragonal group 9 oxo complexes with an oxidation state of IV and higher (and consequently the existence of tetragonal group 10 oxo complexes with an oxidation state of V and higher, and so on), the answer lies in the orbital order and the reactivity of the resulting oxyl species. Interestingly, throughout the analysis this behavior was never observed in any fluoro complex, which is consistent with the successful synthesis of six-coordinate tetragonal metal fluoro complexes with elements beyond group 8.⁴¹

The second observation also explains the tendency of the oxo ligand to form multiple bonds, while the fluoro ligand does not. Linear combination of a $p(X)$ and $d(M)$ atomic orbital results in a set of orbitals where the first can be denoted “ π ”, after its major contributor, or “ π ”, due to its bonding character, and the second can be denoted “ d ” or “ π^* ”. For the sake of the argument, the threshold for an atom-centered orbital denotation was set to 0.75. Orbital populations at X or M above this value were denoted p or d orbitals respectively, orbital populations below this value at X or M were denoted π - or π^* -orbitals, dependent on their symmetry. It is clear that setting such a threshold to change nomenclature is somewhat arbitrary. However, no major conclusions are drawn that depend on the precise value of this threshold. Given that orbitals and populations are not physical observables, a discussion like the one we provide here is of a qualitative, chemical interpretation-oriented nature in the first place.

Choosing Mn as a specific example, Figure 8 compares the shape of one of the two sets of p/π - and d/π^* -type QROs

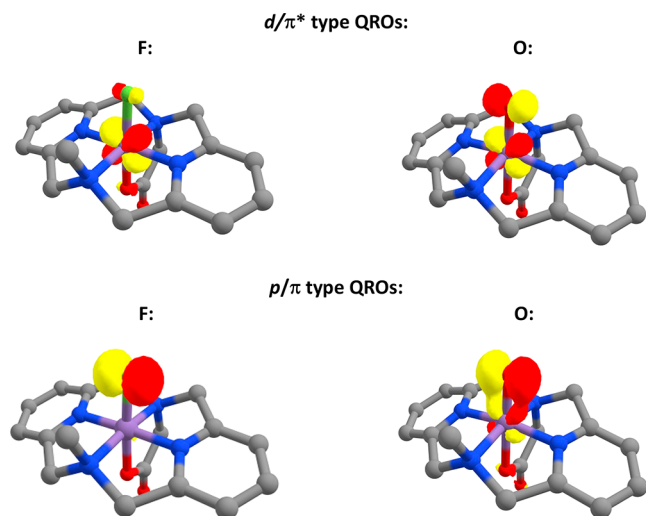


Figure 8. d_{yz}/π_y^* and p_y/π_y QROs of Mn–X complexes for X = F (left) and X = O (right). Hydrogens are omitted for clarity (PBE0-D3/def2-TZVP, iso = 0.1).

between the Mn–F and Mn–O complexes. It becomes obvious that the AO-like p - and d -types of QROs dominate for the Mn–F complex, while the bonding/antibonding π - and π^* -types of QROs dominate the Mn–O complex. This observation explains the tendency of the M–O complexes to form bonds of higher order, especially in those cases where the antibonding π^* -type orbitals are not filled, while the M–F complexes do not have that propensity.

In order to quantify the p/π - and d/π^* -type QRO shapes from Figure 8, Table 2 summarizes the mean Loewdin orbital

Table 2. Mean Loewdin Orbital Populations of p/π and d/π^* QROs of Mn–X Complexes

Loewdin orb. population	X = F	p/π X = O	X = F	d/π^* X = O
$d(\text{Mn})$	0.07	0.23	0.85	0.65
$p(X)$	0.90	0.52	0.05	0.28

populations at Mn and X of the Mn–X complexes for X = F and X = O. On the basis of the specification above, the considered orbitals have been denoted p and d for X = F and π and π^* for X = O. The enhanced π -bonding of the oxo ligand can be attributed to a higher covalency of the Mn–O bond compared to that of the Mn–F bond, which is also reflected in the Mn–X force constants (cf. Figure 4).

AILFT Analysis and AOM Parameters. In order to further quantify the ability of the oxo ligand over the fluoro ligand to form π -bonds with the coordinated metal, an AILFT analysis was performed. The AILFT module in ORCA deduces the d -orbital energies of a metal through the AILFT reconstruction of a CASSCF calculation that leads to a ligand field matrix V^{LFT} that is subsequently diagonalized to yield ligand field orbital energies.^{20,21} From the 15 independent one-electron parameters of the AILFT Hamiltonian (V^{LFT}), one can also extract ligand and metal specific M–L interaction parameters following the angular overlap model (AOM),^{44–46} which can be interpreted as geometry-dependent splitting parameters for individual ligands. Details on the method used to calculate the AOM parameters as well as the full list of calculated parameters can be found in the Supporting Information.

Figure 9 shows a comparison of the d orbital splitting for the Mn–F and Mn–O complexes. While the individual values vary

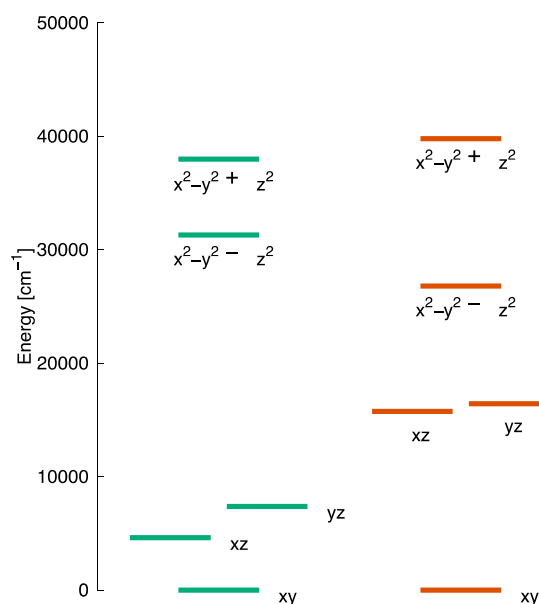


Figure 9. Splitting pattern (d orbital) for Mn–X model complex with X = F (left) and X = O (right).

through the series of evaluated metals, the qualitative picture from Figure 8 is consistent for the other metal complexes as well (for further details see the Supporting Information).

The most striking feature of Figure 9 is certainly the strongly reduced splitting in the t_{2g} set of orbitals for the fluoro ligand. Since the intra- t_{2g} splitting reflects π -bonding, this quantifies the statement that the fluoro ligand is far less involved in π -

bonding than the oxo ligand. From the orbital splitting pattern in Figure 9, one can also see that the d_{xz} and d_{yz} orbitals are not completely degenerate. This is due to the influence of the carboxylate ligand, which imposes anisotropic π -donation. This anisotropic ligation results in an anisotropic trans effect on the X ligand, which while normally of isotropic nature, in turn also becomes anisotropic. Hence, the resulting AOM parameters are not only divided into e_σ and e_π but the e_π parameter is again divided into $e_{\pi s}$ and $e_{\pi c}$. Because the subscripts “s” and “c” stand for “sine” and “cosine” and in spherical coordinate systems the azimuthal angle φ is defined to start at the x axis, $e_{\pi s}$ is defined as the parameter describing the influence of the X ligand on the d_{yz} orbital, and $e_{\pi c}$ is defined as the parameter describing the influence of the X ligand on the d_{xz} orbital. Hence, $e_{\pi s}$ is the parameter influenced more by the anisotropic trans effect of the carboxylate ligand, while $e_{\pi c}$ is expected to pose negligible influences.

Table 3 summarizes the three mean AOM parameters for the fluoro and oxo ligand as well as the individual differences

Table 3. Mean AOM Parameters with Standard Deviations (SD)

X	e_σ [cm ⁻¹]	(SD)	$e_{\pi s}$ [cm ⁻¹]	(SD)	$e_{\pi c}$ [cm ⁻¹]	(SD)
F	15600	(3000)	2000	(1300)	3700	(1300)
O	20400	(6900)	10400	(2700)	13900	(1900)
diff.	4800		8400		10200	

between those two ligands. It is obvious from these values that the σ -donor propensity fluoride is only slightly lower than that of oxygen. However, the key difference is the oxo ligand's ability to form π -bonds, while the fluoride ligand is essentially non- π -bonding despite having occupied orbitals of the correct symmetry. This is reflected by the π -interaction parameters that are 4–5 times lower for the fluoro than for the oxo ligand (see also Figure 8).

Relative Orbital Energies. Because overlap (i.e., spatial interactions) between $p(X)$ and $d(M)$ orbitals is expected to be rather similar for $X = F$ and O , the difference between F and O in the interaction between the $p(X)$ and $d(M)$ orbitals can presumably be attributed to their energy differences. In order to quantify the orbital energy differences, the following model was deployed. The QRO that most resembled a $p(X)$ orbital was located, and the energy relative to the rather nonbonding d_{xy} QRO was determined and cached. The latter orbital energy, $\epsilon_{d_{xy}}$, is assumed to be independent from electronic interactions of the X ligand. For a given metal complex M, the relative energy difference between the $p(F)$ and the $p(O)$ orbital of the proper X ligand was subsequently estimated from the cached values:

$$\begin{aligned}\Delta E_M &= (\Delta p_O - \Delta p_F)_M \\ &= (\epsilon_p - \epsilon_{d_{xy}})_{M-O} - (\epsilon_p - \epsilon_{d_{xy}})_{M-F}\end{aligned}\quad (1)$$

The thus obtained $p(X)$ orbital energy differences are plotted in Figure 10. The value of ΔE states in good approximation for each metal how much deeper the $p(F)$ orbital lies relative to the $p(O)$ orbital. Relative to the nonbonding $d_{xy}(M)$ orbital, most of the $p(F)$ orbitals are found between 2 and 3 eV lower than their $p(O)$ counterparts, with the difference rising up to 3.6 eV. Furthermore, a clear slope can be identified to the right side of the location of the Oxo Wall. This slope can be

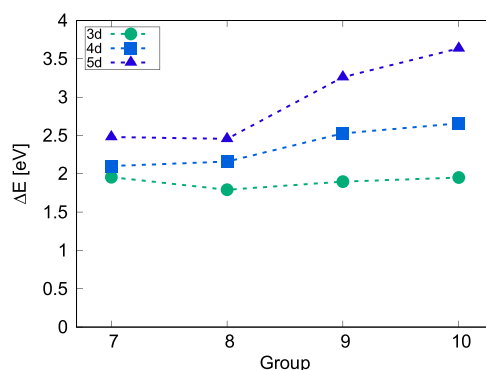


Figure 10. Energy difference of $p(F)$ and $p(O)$ according to eq 1.

attributed to the decreasing interaction between the $p(O)$ and the $d(M)$ orbitals going from group 7 to group 10 oxo complexes as already described above.

Natural Population Analysis and NMR Parameters. We address the final open question, the theoretical explanation of the instability of the closed shell group 10 oxo compounds (i.e. the Pd–O and the Pt–O complexes) through a natural population analysis (NPA), especially for the $p(X)$ orbitals. Even without the significant radical character of the X ligands of the closed shell group 10 M–X complexes, the NPA reveals an electron deficiency especially on the oxo ligands, which after MO theory can be described as a singly bound ligand with a one-electron-equivalent formal charge remaining on the ligand. The NPA impressively shows that the $p_z(O)$ orbitals for the Pd–O and Pt–O complexes, which are the orbitals mostly involved in the M–O σ -bond, lack nearly a full net electron. This makes the oxo ligand a strong electrophile and oxidant, likely resulting in complexes too reactive to be experimentally observed. Overall, the generally decreased population of the $p_z(O)$ orbitals compared to the $p_z(F)$ orbitals is also a strong argument for the rather covalent character of the M–O bond and the more ionic character of the M–F bond, in agreement with the afore-described findings of the orbital analysis. While the latter focused on the M–X π bonds, the NPA findings complement the analysis by addressing the covalency of the σ -bonds between the metals and the X ligands.

In order to correlate the results of the NPA to measurable quantities, NMR shifts of the closed shell complexes were calculated. Table 4 gives the calculated values of the NPA and

Table 4. Calculated NPA and NMR Parameters of Group 10 M–X Complexes

	Ni–X		Pd–X		Pt–X	
	X = F	X = O	X = F	X = O	X = F	X = O
NPA: $\Sigma p(X)^a$	5.640	4.601	5.654	5.019	5.653	5.106
NPA: $p_z(X)$	1.663	1.559 ^b	1.672	1.085	1.670	1.196
NMR: $\delta(X)$ [ppm]	–288.7		–189.0	1251.9	–208.8	632.7

^aSum of NPA values of $p_x(X)$, $p_y(X)$, and $p_z(X)$. ^b $p_y(O) = 1.061$.

of the NMR shifts. Comparing the overall $p(X)$ population (row 1) with the NMR shifts, it becomes obvious that the lack of electron density on the X ligand correlates smoothly with the NMR shifts. This correlation can be explained through the deshielding effect on the nuclei by a less populated $p(X)$ shell.

Comparison of the calculated NMR shifts in Table 4 with experimental data is difficult, because reported NMR shifts are

found on an extremely wide range for both nuclei. ^{19}F NMR shifts of palladium fluoro complexes are typically found in the range of -274 to -323 ppm.^{19,47–50} The example of a palladium difluoride with ^{19}F NMR shifts of -169 and -278 ppm, however, not only shows that the range of shifts is even greater but also shows that they can also drastically differ within the same complex.⁵¹ For platinum fluoro complexes, the range of ^{19}F NMR shifts is even greater and typically spans from -107 to -456 ppm.^{52,53} For nickel fluorides, ^{19}F NMR shifts are typically reported between -251 and -423 ppm.^{54,55} In contrast to the fluoro complexes, the reported oxo complexes are purely hypothetical. Additionally, to the best of our knowledge, ^{17}O NMR shifts of group 10 oxo metal complexes are not reported. ^{17}O NMR shifts of other transition metal oxo complexes are reported between 775 and 1247 ppm.⁵⁶ For comparison, the proposed^{13,57,58} and later retracted¹⁴ late transition metal oxo complexes by Hill et al. had ^{17}O NMR shifts at 570 , 590 , and 605 ppm assigned to palladium and gold oxo complexes and a shift at 330 ppm assigned to a palladium hydroxo complex. All of them were later attributed to the polyoxotungstate ligands. While the calculated values for the fluoro complexes are in decent agreement with measured values of comparable complexes, the calculated values of the hypothetical oxo complexes are beyond the reported range, which is in agreement with the expected instability of the proposed structures.

DISCUSSION

In general,⁵⁹ the linear combination of two heteronuclear atomic orbitals A and B form a bonding/antibonding combination n/n^* , which can be approximately described as

$$n = N_1(A + \alpha B) \quad (2)$$

$$n^* = N_2(B - \alpha A) \quad (3)$$

with N_i being the normalization constants and α being an orbital weighing factor derived from first-order perturbation theory^{60,61} and applied to extended Hückel theory:^{62,63}

$$\alpha \propto \frac{\beta}{\epsilon_A - \epsilon_B} \quad (4)$$

with the resonance integral β and the atomic orbital energies ϵ_i . The Principle of Maximum Overlap^{64–66} simplifies the correlation between the resonance integral β and the (spatial) overlap integral S_{AB} as

$$\beta \propto S_{AB} \quad (5)$$

The expected energy shift of the orbitals $\delta \approx \epsilon_n - \epsilon_A \approx \epsilon_B - \epsilon_{n^*}$ can be approximated as follows:

$$\delta \approx \frac{\beta^2}{\epsilon_A - \epsilon_B} \quad (6)$$

From eqs 2–5, it is obvious that there are two major factors influencing the mixing of orbitals A and B: the orbitals mix more for larger spatial overlap as well as for a smaller difference between the atomic orbital energies. This means that for $S_{AB} \rightarrow 0$ and for $\epsilon_A \ll \epsilon_B$ the values of n and n^* will resemble A and B, respectively (i.e., $\alpha = 0$), rather than a linear combination of A and B, also depicted by the vanishing energy shift of the orbitals as shown in eq 6. While this model is too simplistic to actually derive meaningful values from it, it paints a qualitative

picture that is certainly sufficient to set the values calculated in the “Results” section into context.

In the first approximation (cf. eq 5), the resonance integral β can be treated as proportional to the spatial overlap of orbitals A and B. Due to the reduced charge of the fluoro ligand compared to the oxo ligand, the 1p orbitals of the fluoro ligand are expected to have a smaller radial expectation value than that of the oxo ligand and consequently also a reduced overlap. Indeed, the radial expectation values for the 1p orbitals were calculated as 1.21 and 1.58 Å for fluoride and oxide, respectively. The same trends that are obvious in Figure 4 can be expected to hold for β as well. This result is also consistent with the larger force constants calculated for the group 7 and 8 oxo complexes (cf. Table 1).

The calculated AOM parameters (cf. Table 3) can be interpreted as δ values (cf. eq 6) for different orbital interactions: $e_{\pi c}$ and $e_{\pi s}$ approximately equal δ for the interaction between the $d_{xz}(M)$ and $p_x(X)$, as well as $d_{yz}(M)$ and $p_y(X)$ orbitals, respectively. In addition, the ΔE values from Figure 10 (derived from eq 1) exactly quantify the difference between $X = \text{F}$ and $X = \text{O}$ as $\epsilon_{p(X)} - \epsilon_{d(M)}$. Hence, it can be directly deduced from these ΔE values that assuming a comparable β the δ values for $X = \text{F}$ are expected to be smaller than those for $X = \text{O}$ (because the denominator in eq 6 is bigger for $X = \text{F}$), which agrees with the AOM parameters.

Comparing eqs 4 and 6, one would expect a trend for α similar to that for δ . Indeed, comparing the mean Loewdin orbital populations from Table 2 (depicted in Figure 8), one can see that the orbital mixing between the $p(X)$ and $d(M)$ orbitals is much smaller for $X = \text{F}$ than for $X = \text{O}$. This is the direct consequence of a smaller α value in eq 2, resulting from the larger orbital energy difference in eq 4 for $X = \text{F}$ than for $X = \text{O}$.

The $p(\text{F})$ orbital has a lower energy than the $p(\text{O})$ orbital due to the higher effective nuclear charge experienced by the 2p electrons for fluorine since the increased nuclear charge of the fluorine nucleus is incompletely shielded by the other electrons. The difference of the p orbital energy between F and O has implications for the analyzed fluoro and oxo complexes: While the $p(\text{F})$ orbitals simply remain inaccessible for multiple bonding, the $p(\text{O})$ orbitals are so exposed that if not stabilized through $d(M)$ interactions then a singly bound oxo ligand would be extremely reactive and hence unstable. In some instances met in our calculations, the oxidation potential of the metal center is already high enough to draw an electron out of a $p(\text{O})$ orbital, resulting in an oxyl radical complex. The NPA of the $p_z(\text{O})$ orbitals in Table 4 reveals that the oxo ligands in the hypothetical Pd–O and Pt–O complexes are so electron-deficient that they will likely react with even extremely weak electron donors by oxidation or oxygenation. Potential stabilization of those complexes by more electron-donating ligands to shift the electrons more toward the oxo ligand will instead result in increased basicity, eventually leading to already well-known and studied hydroxyl complexes (and probably deprotonated solvent).

Synthetically, we can think of two ways in which these results can be utilized. First, the energetic mingling of the d manifold and the $p(\text{O})$ orbitals observed for the group 9 and 10 oxo complexes leads to the formation of oxyl radical complexes in some cases. Tweaking the electronic properties of the ligand (e.g., by adding electron-withdrawing substituents like F, CF_3 , or NO_2 to the pyridyl moieties) can potentially lead to an energetic stabilization of the d manifold, possibly

strong enough to form oxyl radical complexes with group 8 or even group 7 metals. Further fine-tuning could eventually lead to “designer complexes” with oxyl character, potentially exhibiting unprecedented (catalytic) properties. Second, although chemically extremely challenging, we consider pushing the limits to a point where a late transition metal d manifold can be stabilized by extremely electron-withdrawing ligands to an extent where chemically meaningful interactions with the p(F) orbitals are possible, practically resulting in M–F multiple bonding. However, to date this has admittedly never been observed experimentally. The targeted search for such unusual compounds is, however, at the heart of chemical curiosity.

CONCLUSIONS

Through an extensive computational analysis of the geometric and electronic structure of a series of model complexes around the Oxo Wall, we solidified the theoretical foundation of the Oxo Wall concept. We have shown that the p orbitals of oxo ligands are energetically more readily accessible than the p orbitals of fluoro ligands by more than 2 eV. This leaves the fluoro ligand practically inaccessible for multiple bonding and the oxo ligand too reactive for formation of stable complexes with a singly bound oxo species. Hence, we conclude that there is no theoretically justifiable or practically meaningful concept of a Fluoro Wall. While the present analysis mostly focused on π -bonding, AOM and NPA analyses suggest that differences in σ -bonding also play a crucial role. According to our analysis, the M–F σ -bond seems to possess a rather ionic character, while the M–O σ -bond is of a more covalent nature, which is likely the source of the high electrophilicity and oxidative power of the oxo-complexes beyond the Oxo Wall, resulting in their practical instability. However, further research is required to evaluate the subtle differences in detail.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.inorgchem.9b03474>.

Complete spin state analysis, Cartesian coordinates of all geometry optimized model structures, force constants, and full AILFT analysis, including AOM parameters (PDF)

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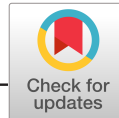
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A1.3 “All-electron scalar relativistic basis sets for the elements Rb–Xe”^[4]



FULL PAPER

All-electron scalar relativistic basis sets for the elements Rb–Xe

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Abstract

Segmented all-electron relativistically contracted (SARC) basis sets are presented for the elements $_{37}\text{Rb}$ – $_{54}\text{Xe}$, for use with the second-order Douglas–Kroll–Hess approach and the zeroth-order regular approximation. The basis sets have a common set of exponents produced with established heuristic procedures, but have contractions optimized individually for each scalar relativistic Hamiltonian. Their compact size and loose segmented contraction, which is in line with the construction of SARC basis sets for heavier elements, makes them suitable for routine calculations on large systems and when core spectroscopic properties are of interest. The basis sets are of triple-zeta quality and come in singly or doubly polarized versions, which are appropriate for both density functional theory and correlated wave function theory calculations. The quality of the basis sets is assessed against large decontracted reference basis sets for a number of atomic and ionic properties, while their general applicability is demonstrated with selected molecular examples.

KEYWORDS

basis sets, DKH, scalar relativistic Hamiltonians, ZORA

1 | INTRODUCTION

Consideration of the effects of relativity is an important aspect in the theoretical modeling of chemical systems.^[1–7] At the all-electron level, relativistic effects are included in quantum chemical calculations through various levels of approximation to the fully relativistic four-component Dirac Hamiltonian. The latter can be reduced^[8,9] exactly or approximately to a quasi-relativistic two-component Hamiltonian following various different formalisms.^[5,6] Additionally, spin-dependent terms may be eliminated in these Hamiltonians to provide spin-free scalar relativistic formulations. Among the most popular approximations that have been extensively implemented in quantum chemistry packages and find wide use even in nonspecialist applications of quantum chemistry are the Douglas–Kroll–Hess (DKH) method,^[10–16] the zeroth-order regular approximation (ZORA),^[17–19] and the exact-2-component approach (X2C).^[20–27]

Each quasi-relativistic approach presents distinct requirements with respect to the design and construction of the basis sets used in molecular quantum chemistry calculations, a consideration additional to the appropriateness of a given basis set for the type of electronic structure method and, occasionally, for the targeted property.^[28,29] As a result, several families of all-electron basis sets exist and more are being actively developed, that attempt to address these combined requirements in an optimal and balanced way. In recent years, we have been developing a family of segmented all-electron relativistically contracted (SARC)^[30–34] basis sets for routine calculations, chiefly based on density functional theory (DFT), in combination with two widely available scalar relativistic Hamiltonians, namely the second-order Douglas–Kroll–Hess (DKH2)^[10–16] and the ZORA.^[17–19] The construction of the basis sets follows simple rules and strives to provide a reasonable compromise between accuracy and efficiency. The SARC basis sets have already been used extensively in hundreds

of applications and represent the main options for DKH2 and ZORA calculations in the popular ORCA program package.^[35,36] The SARC family so far covers elements past Xe and up to Lr.^[30–34] For their combination with lighter atoms we proposed Hamiltonian-specific reconstructions of all-electron nonrelativistic Karlsruhe basis sets.^[37] This was deemed sufficient for elements up to Kr and the corresponding recontracted versions are available in ORCA as DKH-def2- or ZORA-def2-basis sets. However, no satisfying solution existed so far for the elements Rb–Xe, for which recontracted primitives from small nonrelativistic Ahlrichs–May basis sets^[38] were used as a temporary solution. These basis sets were very weakly polarized and their construction and range of exponents were far from optimal for use with scalar relativistic Hamiltonians in combination with modern quantum chemical methods. This deficiency is particularly crucial for the chemically important 4d transition metals. Here we propose a series of DKH2 and ZORA SARC basis sets developed from the ground up for the fifth-row elements Rb–Xe.

The new basis sets maintain the segmented and loosely contracted design of previous SARC basis sets.^[30–34] Exponents were obtained with an even-tempered progression and were contracted individually for the DKH2 and ZORA Hamiltonians and the final set of primitives was adapted to the different requirements of the *s*, *d*, and *p* blocks based on the chemical nature of the included elements. The basis sets are equivalent to triple-zeta quality and can be combined with the other members the SARC family as well as with the recontracted^[30] def2 basis sets^[37] for elements up to Kr. The generated basis sets are complemented with one set of polarization functions (–P) for methods like DFT as well as with a more extensive set of correlation functions (–PP) for common wave function based post-Hartree–Fock methods. The new SARC basis sets are evaluated for a range of atomic and molecular properties and shown to combine good accuracy while maintaining a reasonable size that facilitates their use in realistic applications. All SARC basis sets are provided in input format as Supporting Information and are included in the basis set library of the ORCA program package.^[35]

2 | CONSTRUCTION OF BASIS SETS

Following the well-described procedure for the generation of SARC basis sets,^[30–34] the starting point was the determination of the radial expectation values of the innermost orbitals for every angular momentum quantum number. These values were used as generator functions for producing an even-tempered series of primitive Gaussian functions for each angular momentum, as described previously^[30–33] and summarized below. The initial radial expectation values were obtained from atomic ground-state restricted open-shell Hartree–Fock (ROHF) calculations, following the Stavrev–Zerner spin-averaged (SA) formalism.^[39] The SA-ROHF is a variant of Zerner's configuration-averaged (CA) formalism,^[40] that averages over all states with not only a given configuration, but also a given spin, which leads to the production of degenerate orbitals. Exponents from the universal Gaussian basis set (UGBS) by de Castro and Jorge^[41] were

utilized to generate a sufficiently large, completely decontracted (29s21p17d) basis set as reference for benchmark calculations. In the following, “UGBS” refers to this extended basis set, comprising 177 functions per atom. For the assessment of the innermost radial expectation values ($\langle r_l \rangle$), as well as for property calculations, the DKH2 scalar relativistic Hamiltonian was employed.

All atoms were considered in their atomic ground states. These are the following, including their atomic valence electron configurations: Rb (2S , $5s^1$), Sr (1S , $5s^2$), Y (2D , $4d^15s^2$), Zr (3F , $4d^25s^2$), Nb (6D , $4d^45s^1$), Mo (7S , $4d^55s^1$), Tc (6S , $4d^55s^2$), Ru (5F , $4d^75s^1$), Rh (4F , $4d^85s^1$), Pd (1S , $4d^{10}$), Ag (2S , $4d^{10}5s^1$), Cd (1S , $4d^{10}5s^2$), In (2P , $4d^{10}5s^25p^1$), Sn (3P , $4d^{10}5s^25p^2$), Sb (4S , $4d^{10}5s^25p^3$), Te (3P , $4d^{10}5s^25p^4$), I (2P , $4d^{10}5s^25p^5$), and Xe (1S , $4d^{10}5s^25p^6$). The resulting innermost radial expectation values ($\langle r_l \rangle$) for the 1s, 2p, and 3d orbitals are listed in Table 1.

From the SA-ROHF/UGBS radial expectation values, we derived the generator exponents α_l of the tightest *s*, *p*, and *d* functions following a previously described procedure according to:

$$\alpha_l = k_l \frac{2 f_l^2}{\pi \langle r_l \rangle^2}$$

The factor f_l is 1, 4/3, and 8/5 for *l* = *s*, *p*, and *d*, and k_l is an empirically adjustable scaling factor that defines the magnitude of the tightest exponent for each angular momentum. For the present case of the elements Rb–Xe, k_l was set to 2000, 250, and 50 for *s*, *p*, and *d* functions, respectively. These values were found in test atomic calculations to produce exponents sufficiently high to be appropriate for

TABLE 1 Radial expectation values of innermost orbitals (in Bohr) determined from spin-averaged DKH2-ROHF calculations with the UGBS basis set

Element	$\langle r_s \rangle$	$\langle r_p \rangle$	$\langle r_d \rangle$
Rb	0.039830	0.154925	0.522941
Sr	0.038688	0.150204	0.496413
Y	0.037603	0.145748	0.472567
Zr	0.036571	0.141537	0.451126
Nb	0.035588	0.137550	0.431615
Mo	0.034650	0.133770	0.413899
Tc	0.033755	0.130180	0.397817
Ru	0.032898	0.126767	0.382946
Rh	0.032079	0.123518	0.369255
Pd	0.031293	0.120421	0.356409
Ag	0.030540	0.117467	0.344603
Cd	0.029817	0.114644	0.333575
In	0.029122	0.111943	0.323245
Sn	0.028453	0.109358	0.313544
Sb	0.027810	0.106880	0.304413
Te	0.027189	0.104503	0.295800
I	0.026591	0.102221	0.287664
Xe	0.026014	0.100027	0.279964

the scalar ZORA and DKH2 relativistic Hamiltonians, without being so high as to create the potential for grid-related numerical instabilities in DFT calculations.^[28] As discussed previously,^[30–33] keeping these values constant across a row of the periodic table is a pragmatic choice to enable straightforward construction of a complete basis set family, in line with the philosophy of simplicity followed in the construction of the SARC basis sets. The resulting maximum exponents are given in Table 2.

Subsequently, the basis set primitives were constructed in an even-tempered fashion using the series $\alpha_i \cdot \chi_i^{-i}$ ($i = 1, 2, 3, \dots$) with the parameter χ_i set to 2.25, 2.50, and 2.80 for $l = s, p$, and d , respectively. This parameter controls the spacing of one primitive function from the next one, that is, the ratio between successive Gaussian exponents. The termination of the series is controlled by a cutoff value σ set individually for every atom to $\sigma = Z \cdot n_l$ with Z being the atomic number and n_l ($l = s, p$, and d) being a cutoff parameter calibrated individually for the s, p , and d block elements (see Table 3). This defines the most diffuse exponent for each angular momentum. Collectively, therefore, the above parameters define the total number of primitive functions that are generated for each angular momentum. The above values were selected empirically by a combination of testing with respect to atomic properties for selected elements relative to the UGBS reference and by taking into account approximate target sizes for each angular momentum subspace. The latter approximate targets are used as an important constraint because we require the new basis sets to be compatible in usage with the existing SARC basis sets for elements heavier than Xe and with the recontracted def2 all-electron basis sets for elements lighter than Rb, and hence intermediate in size.

TABLE 2 Maximum exponents per angular momentum α_l (in Bohr⁻²) used in the SARC basis sets

Element	α_s	α_p	α_d
Rb	802,582.167241	11,788.392711	297.978347
Sr	850,663.033114	12,541.070472	330.676856
Y	900,461.459177	13,319.637239	364.891134
Zr	951,998.900662	14,123.997520	400.400284
Nb	1,005,316.833948	14,954.655585	437.418386
Mo	1,060,482.828479	15,811.757705	475.665155
Tc	1,117,464.908547	16,695.870613	514.900622
Ru	1,176,443.639667	17,606.992511	555.667527
Rh	1,237,281.375224	18,545.438347	597.636788
Pd	1,300,216.635828	19,511.611774	641.494250
Ag	1,365,123.846655	20,505.286897	686.202008
Cd	1,432,129.293106	21,527.566722	732.323723
In	1,501,300.826074	22,578.948957	779.877626
Sn	1,572,729.347489	23,659.005588	828.882754
Sb	1,646,296.826083	24,768.785640	879.353917
Te	1,722,358.882847	25,908.369888	931.308900
I	1,800,697.570348	27,078.048041	984.734293
Xe	1,881,463.713587	28,278.939416	1,039.646541

From the resulting uncontracted basis set, which is the same for both scalar relativistic Hamiltonians, the innermost eight s , six p , and five d functions were then contracted to contracted Gaussian-type functions (CGTFs). This was found to be the maximum acceptable number of contracted primitives that results in acceptable contraction errors compared to the UGBS reference. In line with the existing SARC basis sets, no other contraction is employed. An augmented diffuse function of p type is added for the valence space of the $5p$ block elements to account for their potential (partially) anionic character in molecular and ionic calculations. Contraction coefficients were optimized for ZORA and DKH2 scalar relativistic Hamiltonians separately in order to account for the differences in relativistic treatment of the innermost electrons by the two approximations.^[28] An example of the differences produced by the two Hamiltonians on the s orbitals of Cadmium is provided in Figure S1 of the Supporting Information. In view of the number of functions used to describe the valence space of the neutral and most common ionic configurations of the elements, the resulting SARC basis sets can be considered of triple- ζ quality, although the highly uncontracted nature of the basis sets makes this nomenclature rather imprecise. The utilization of five d functions for Y–Cd formally exceeds the triple- ζ designation but is in line with other recently proposed all-electron basis sets for these elements.^[42] The cutoff parameters n_l , as well as the final size and contraction pattern of the new SARC basis sets are summarized in Table 3.

As additional polarization functions, we opted for a conservative DFT-oriented approach in the definition of SARC-TZVP. For d block elements, scaling the sum of the two most diffuse d functions by 1.93 generated a set of f functions, while for p block elements the outermost d function was scaled by 1.43 to generate a set of f primitives. Additional polarization/correlation functions (SARC-TZVPP) were generated as follows, guided by maximizing the correlation energy recovered in test CCSD(T) calculations: for s block elements, an additional set of f primitives was generated by scaling the sum of the last two d functions by 1.59. For p block elements, two sets of f primitives were generated by scaling the average of the two most diffuse d functions by 0.69 and 4.41. For d block elements, the sum of the two outer d functions was scaled by 0.98 and 3.48 for two sets of f primitives and 2.13 for an extra set of g primitives. The d block elements were additionally augmented with a diffuse d primitive, consecutively following the generation procedure described above. For optimal balance, the combination of the presented basis sets is recommended with the already published SARC basis sets for heavier elements and the ZORA or DKH2 recontracted all-electron def2-TZVP basis sets for lighter elements in molecular calculations.

3 | ASSESSMENT OF BASIS SETS

In this section, the performance of the new SARC basis sets is assessed for selected properties. Atomic properties were calculated without additional polarization functions (SARC-TZV) to enable direct comparison and evaluation of incompleteness errors against the large

TABLE 3 Cutoff parameters n_l for s , p and d block elements, used in the generation of the SARC basis sets, and the resulting size (number of functions) and pattern of the corresponding uncontracted (U-SARC) and (contracted) SARC basis sets

Elements	n_s	n_p	n_d	U-SARC size	SARC-TZV size
s block	0.0018	0.0018	0.005	112 (22s15p9d)	70 [15s10p5d]
d block	0.0018	0.0018	0.005	112 (22s15p9d)	70 [15s10p5d]
p block	0.0018	0.0010	0.005	115 (22s16p9d)	73 [15s11p5d]

TABLE 4 Estimated incompleteness and contraction errors (E_h) from comparison of the UGBS with uncontracted (U-SARC) and contracted SARC-TZV basis sets using spin-averaged ROHF calculations with the DKH2 Hamiltonian

Element	UGBS	U-SARC	SARC	ΔE_{incomp}	$\Delta E_{\text{contr.}}$
Rb	−2,978.882826	−2,978.807987	−2,978.801387	0.074839	0.006600
Sr	−3,177.042664	−3,176.959874	−3,176.952455	0.082790	0.007420
Y	−3,382.596729	−3,382.503930	−3,382.495565	0.092799	0.008365
Zr	−3,595.790955	−3,595.687277	−3,595.677825	0.103678	0.009452
Nb	−3,816.829093	−3,816.712366	−3,816.701612	0.116727	0.010754
Mo	−4,045.740938	−4,045.610935	−4,045.598771	0.130003	0.012164
Tc	−4,282.473586	−4,282.329671	−4,282.315980	0.143915	0.013691
Ru	−4,527.359444	−4,527.198159	−4,527.182679	0.161285	0.015480
Rh	−4,780.464841	−4,780.285780	−4,780.268289	0.179061	0.017491
Pd	−5,041.903747	−5,041.702055	−5,041.682252	0.201692	0.019803
Ag	−5,311.865066	−5,311.645843	−5,311.623497	0.219223	0.022346
Cd	−5,590.255633	−5,590.015344	−5,589.990086	0.240289	0.025258
In	−5,877.040384	−5,876.780360	−5,876.751755	0.260024	0.028605
Sn	−6,172.404077	−6,172.117660	−6,172.085350	0.286417	0.032310
Sb	−6,476.450405	−6,476.136315	−6,476.100013	0.314090	0.036302
Te	−6,789.178209	−6,788.835449	−6,788.794887	0.342760	0.040562
I	−7,110.789125	−7,110.415776	−7,110.370708	0.373349	0.045068
Xe	−7,441.394819	−7,440.988867	−7,440.939047	0.405952	0.049820

UGBS reference. Molecular properties were calculated with the inclusion of polarization functions for transition metals (SARC-TZVP), while all post-Hartree–Fock calculations reported here were performed with additional correlation functions (SARC-TZVPP). Lighter elements were equipped with relativistically recontracted def2-TZVP basis sets for Hartree–Fock and DFT, and with relativistically recontracted def2-TZVPP basis sets for correlated wave function based methods.

3.1 | Atomic properties

The assessment of the internal consistency and construction quality of the newly generated SARC basis sets began with SAHF calculations of the atomic ground states. The resulting energies were compared to energies obtained with the fully uncontracted SARC (U-SARC) basis sets as well as the UGBS basis sets in order to determine both the estimated incompleteness error and the contraction error. All ground state absolute energy values for the fifth period elements and incompleteness and contraction errors are given in Table 4. Both errors rise monotonically, the latter between 6.6 mE_h for Rubidium and 50 mE_h for Xenon and the former between 75 mE_h for Rubidium and 406 mE_h for Xenon. The overall

deviation of the total energy from the values obtained with UGBS basis sets stays below 0.5 E_h for the whole SARC series, which compares very favorably with corresponding values for heavier elements. As an indication of the impact on the computational cost, the total run time for the calculation of the Rh ground state energy on 1 CPU is reduced from 5 min and 4 s (UGBS) to 23 s (U-SARC) and the consecutive introduction of contraction reduces the run time further down to 11 s (SARC).

A more detailed measure of basis set performance for atomic systems is found by comparison of all orbital energies and radial expectation values between the results obtained with UGBS basis set and the results obtained with the newly generated SARC basis set. Xenon was chosen as a representative example, because the proper representation of its innermost orbitals has the highest requirements on the CGTFs, and hence the biggest deviation in the energies of the innermost orbitals from the values obtained with the UGBS basis set was expected—and observed—for Xenon. The deviation in the calculated orbital energies for Xenon does not exceed 71 mE_h and practically disappears in the valence region. The radial expectation values are in extremely good agreement, with practically identical results in the core region and deviations in the valence region staying well below 0.1 pm (0.0019 Bohr). All orbital energies and radial expectation

	UGBS		SARC		ΔE	$\Delta \langle r \rangle$
	E	$\langle r \rangle$	E	$\langle r \rangle$		
1s	-1,275.1970	0.0260	-1,275.2533	0.0260	-0.0563	0.0000
2s	-202.2477	0.1139	-202.3150	0.1139	-0.0673	0.0000
2p	-181.4455	0.1000	-181.517	0.1000	-0.0711	0.0000
3s	-42.9723	0.3047	-43.0106	0.3047	-0.0382	0.0000
3p	-36.0620	0.3028	-36.0943	0.3029	-0.0324	0.0001
3d	-25.7330	0.2800	-25.7613	0.2801	-0.0283	0.0001
4s	-8.4230	0.7175	-8.4371	0.7172	-0.0141	-0.0003
4p	-6.1322	0.7647	-6.1406	0.7647	-0.0084	0.0000
4d	-2.6659	0.8762	-2.6645	0.8778	0.0015	0.0016
5s	-1.0090	1.9058	-1.0102	1.9047	-0.0012	-0.0012
5p	-0.4563	2.3139	-0.4566	2.3142	-0.0002	0.0003

TABLE 5 Orbital energies (E_h) and radial expectation values (Bohr) for Xenon: Comparison between UGBS and SARC-TZV basis sets from HF calculations with the DKH2 Hamiltonian

Element	UGBS			SARC			Expt. ^[45]		
	IP ₁	IP ₂	IP ₃	IP ₁	IP ₂	IP ₃	IP ₁	IP ₂	IP ₃
Rb	4.26	27.41	-	4.24	27.41	-	4.18	27.29	-
Sr	5.68	11.20	-	5.68	11.20	-	5.69	11.03	-
Y	6.30	12.24	20.70	6.30	12.25	20.71	6.22	12.24	20.52
Zr	6.51	13.22	23.32	6.49	13.23	23.31	6.63	13.13	22.99
Nb	6.84	14.25	25.29	6.78	14.24	25.29	6.76	14.32	25.04
Mo	7.15	16.18	27.16	7.11	16.17	27.15	7.09	16.16	27.13
Tc	7.03	15.30	29.75	7.15	15.31	29.73	7.28	15.26	29.54
Ru	7.51	16.96	28.56	7.47	16.95	28.56	7.36	16.76	28.47
Rh	7.63	18.31	31.21	7.59	18.30	31.20	7.46	18.08	31.06
Pd	8.64	19.62	33.10	8.44	19.62	33.09	8.34	19.43	32.93
Ag	7.81	21.76	34.94	7.77	21.75	34.93	7.58	21.49	34.83
Cd	8.99	17.26	37.71	8.99	17.28	37.70	8.99	16.91	37.48
In	5.57	18.94	-	5.57	18.95	-	5.79	18.87	-
Sn	7.19	14.23	-	7.20	14.24	-	7.34	14.63	-
Sb	8.86	16.43	-	8.87	16.44	-	8.61	16.53	-
Te	8.77	18.67	-	8.77	18.68	-	9.01	18.60	-
I	10.55	18.76	-	10.55	18.78	-	10.45	19.13	-
Xe	12.40	21.11	-	12.41	21.12	-	12.13	21.21	-

TABLE 6 B3LYP-DKH2 results with the SARC-TZV and UGBS basis sets for the first, second, and third ionization potentials (in eV) for Rb–Xe

values for Xenon with UGBS and SARC basis sets as well as their differences are given in Table 5 (see Supporting Information Table S2 for corresponding B3LYP orbital energies).

The representation of the valence orbitals is a good indicator of the accuracy of a given basis set, but ionization potentials (IPs) and electron affinities (EAs) calculated at the DFT level give a more detailed insight into the practical applicability of the new SARC basis sets. Comparison of the first two IPs for all fifth period elements and additional third IP for second row transition metals calculated with the B3LYP functional^[43,44] show an overall good agreement between the values calculated with UGBS and SARC basis sets (Table 6). Most of the deviations lie below 0.05 eV, never exceeding 0.20 eV. The

experimental values are provided for reference, but we note that the better agreement in some cases of the IPs calculated with SARC basis sets with experiment compared to those calculated with UGBS basis sets should not be read as more than accidental, given that the complete basis set limit of the method might still not be captured by UGBS and that the experimental values incorporate effects that are ignored in the present calculations, such as spin-orbit coupling.

Due to the increase in electronegativity, EAs, which require a proper electronic description of anionic states, become increasingly important down the row. Hence, *p* block elements were equipped with an additional diffuse *p* function to account for this requirement. The resulting EA values, in analogy to the IP values given above, can

TABLE 7 B3LYP-DKH2 electron affinities (in eV) for In–I with the UGBS and SARC-TZV basis sets

Element	UGBS	SARC	Expt. ^[46–50]
In	0.24	0.34	0.38
Sn	1.22	1.26	1.11
Sb	0.94	0.97	1.05
Te	2.06	2.07	1.97
I	3.27	3.28	3.06

be found in Table 7. Again, most of the deviations between the results obtained with SARC and UGBS basis sets lie below 0.05 eV.

All the above examples are reported with the DKH2 Hamiltonian. Supporting Information Tables S1, S3, and S4 provide the corresponding ZORA versions of Tables 5, 6, and 7. The ZORA results are perfectly in line with the conclusions drawn above on the basis of the DKH2 calculations.

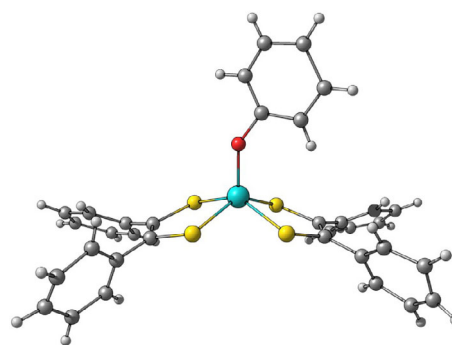
To analyze how the newly generated SARC basis sets perform with post-Hartree–Fock methods, the EA of iodine was also assessed through CCSD(T) calculations with the SARC basis set, augmented with the correlation functions introduced above, as well as with the corresponding DKH-optimized basis sets from the correlation-consistent basis set family.^[51] The calculation with the DKH2 version of SARC-TZVPP yielded an EA for iodine of 3.02 eV, while employing the series of cc-pVTZ-DK, aug-cc-pVTZ-DK, and cc-pVQZ-DK basis sets resulted in EA values of 2.91, 3.19, and 3.23 eV, respectively (the reported experimental value^[50] is 3.06 eV). Another example that demonstrates the accuracy and efficiency of the newly generated SARC basis set is the calculation of the excitation energy of Zr from its ($4d^2 5s^2$, $S = 1$) ground state to its ($4d^3 5s$, $S = 2$) state (experimental value reported as $5,541\text{ cm}^{-1}$).^[52] The corresponding DKH2 CCSD(T) calculation with SARC-TZVPP yielded an excitation energy of $5,077\text{ cm}^{-1}$ while the same calculation with the cc-pVTZ-DK basis set^[53] gave an excitation energy of $4,278\text{ cm}^{-1}$. The SARC-TZVPP basis sets were found to recover more correlation energy in these calculations compared to the correlation-consistent basis sets, a result that might be in part related to the greater number of uncontracted functions and in part to the tighter exponents for the high angular momentum functions used in the SARC basis sets. We acknowledge that correlated wave function calculations are not the principal domain of intended application for the SARC basis sets. Other basis sets, usually incorporating general contractions, have been proposed specifically for such calculations^[51,53–61] and they often also offer the possibility of basis set extrapolation through a systematically converging series. Nevertheless, the above observations suggest that in their TZVPP version the SARC basis sets are sufficiently flexible to be used in routine wave function based calculations.

3.2 | Molecular applications

This section presents selected examples relating to molecular applications and includes comparisons of the SARC basis sets with other basis sets available in the literature. Assessment of molecular properties with

TABLE 8 Bond lengths r (Å) and dissociation energies D_e (eV) of strontium, silver, and (homonuclear) iodine diatomics computed with the PBE0 density functional and the DKH2 Hamiltonian, without and with BSSE counterpoise corrections (CPC)

	SARC-TZVP		SARC-TZVP+CPC		Δr	ΔD_e
	r	D_e	r	D_e		
SrH	2.136	1.79	2.136	1.79	0.000	0.00
SrO	1.905	4.06	1.905	4.05	0.000	−0.01
SrF	2.080	5.39	2.080	5.38	0.000	−0.01
AgH	1.623	2.27	1.623	2.26	0.000	−0.01
AgO	1.931	0.76	1.931	0.74	0.000	−0.02
AgF	1.987	3.22	1.987	3.20	0.000	−0.02
I ₂	2.663	2.03	2.663	2.02	0.000	−0.01

**FIGURE 1** Structure of $[\text{Mo}^{\text{IV}}(\text{OPh})(\text{S}_2\text{C}_2\text{Ph}_2)_2]^-$ ^[64] [Color figure can be viewed at wileyonlinelibrary.com]

the new SARC basis sets starts with representative analyses of basis set superposition error (BSSE) with the counterpoise correction method by Boys and Bernardi.^[62] The potential energy surfaces of selected diatomic molecules were scanned using the PBE0 hybrid functional^[63] with the DKH2 Hamiltonian. The optimized bond lengths and the dissociation energies of all dimers with and without the counterpoise correction, as well as their differences, are summarized in Table 8. The deviation of dissociation energies with and without CPC is generally found between 0.01 and 0.02 eV, while the deviation in bond length is essentially zero. The comparison leads to the conclusion that there are no significant BSSE effects in the valence space to be expected from the new SARC basis sets in molecular DFT calculations.

As another test case, we use a transition metal complex to compare the effect of the choice of method on geometry optimization. Figure 1 shows the structure of the complex $[\text{Mo}^{\text{IV}}(\text{OPh})(\text{S}_2\text{C}_2\text{Ph}_2)_2]^-$, a molybdenum system reported by Lim and Holm^[64] as a biomimetic analogue for the active site of Mo-containing enzymes that comprises two chelate phenyl-substituted dithiolenes and a phenoxy group.

Crystallographic coordinates of the complex (ID: IDELUY) were used as the starting point for DFT geometry optimizations with the BP86 functional.^[65,66] Increased integration grids were applied throughout (Grid6 in ORCA nomenclature). Table 9 compares the Mo–O and Mo–S bond

TABLE 9 Optimized Mo–O and Mo–S (averaged) bond lengths (in Å) for $[\text{Mo}^{\text{IV}}(\text{OPh})(\text{S}_2\text{C}_2\text{Ph}_2)_2]^-$ using different Mo basis sets and Hamiltonian combinations

Method	Mo–O	Mo–S
Expt.	1.886	2.326
def2-TZVP	1.908	2.327
def2-TZVPP	1.906	2.327
ZORA/SARC-ZORA-TZVP	1.912	2.329
ZORA/SARC-ZORA-TZVPP	1.909	2.328
DKH2/SARC-DKH-TZVP	1.879	2.250
DKH2/SARC-DKH-TZVPP	1.882	2.257

Note: All results were obtained with the BP86 functional and all-electron def2-TZVP basis sets for ligand atoms, either in their nonrelativistic^[37] or relativistically recontracted versions as appropriate. The “AutoAux” procedure of ORCA was used for the generation of auxiliary basis sets when needed^[67] and the “DKH1CAutoAux” setting was activated for geometry optimizations with the DKH2 Hamiltonian.

lengths obtained with a different basis sets for Mo and different scalar relativistic Hamiltonians, specifically the def2-TZVP and def2-TZVPP basis sets that employ an effective core potential (ECP) replacing the inner 28 electrons of Mo^[68] (corresponding valence space contractions are $[6s4p3d1f]$ and $[6s4p3d2f1g]$, respectively),^[37] and the new SARC basis sets with the ZORA and the DKH2 approaches. Optimizations that use the ECP basis set for Mo and the SARC-ZORA all-electron calculations provide almost indistinguishable results, approximating the crystallographic parameters equally well. This is a nice indication that the two approaches can be used interchangeably for geometry optimizations. DKH2 calculations provide slightly shorter Mo–O bonds but on the other hand they also yield rather too short Mo–S bond lengths. ZORA calculations proved robust and neither required nor were they affected by further increase in radial integration accuracy. In contrast, this had a beneficial effect on the stability and rate of convergence of DKH2 calculations, albeit increasing at the same time the computational cost. Interestingly, even though the ECP-based calculations had an advantage in terms of the time required to complete the self-consistent-field procedure owing to the smaller total number of basis functions, the ZORA all-electron optimizations either with the SARC-TZVP or the SARC-TZVPP basis sets were always the fastest calculations for the present complex because they consistently required the least optimization steps to converge to the minimum. It is noted that in cases when ZORA turns out to be the preferred all-electron scalar relativistic approach, as for the present system, the SARC basis sets may currently be the only choice for quantum chemistry programs that use Gaussian-type basis sets, as the only other ZORA-specific option known to us are the Slater-type basis sets of Van Lenthe and Baerends.^[69]

A different type of application concerns the analysis of valence orbitals in transition metal complexes on the basis of multireference calculations. As a test case, we use the MoOCl_5^{2-} complex and demonstrate the results of ab initio ligand field theory (AILFT) analysis^[70] of its d manifold based on complete active space SCF (CASSCF) calculations. Table 10 summarizes the results obtained using the SARC basis sets for Mo (CASSCF calculation with the DKH2 Hamiltonian) and compares the produced values to those obtained with the standard ECP-based def2-TZVP and def2-TZVPP basis

TABLE 10 Comparison of basis sets for the ab initio ligand field theory (AILFT) analysis of the d manifold of MoOCl_5^{2-} (energies relative to d_{xy} in cm^{-1}) from CASSCF calculations

Mo basis set	d_{xy}	d_{xz}/d_{yz}	$d_{x^2-y^2}$	d_{z^2}
def2-TZVP	0	14,300	22,290	45,290
def2-TZVPP	0	14,290	22,180	45,270
SARC-DKH-TZVP	0	14,160	22,010	44,840
SARC-DKH-TZVPP	0	14,150	22,000	44,770
Sapporo-DKH-TZP	0	14,130	21,840	44,760
cc-pVTZ-DK	0	14,150	21,920	44,750
Jorge-TZP-DKH	0	15,260	33,230	31,760
Expt. ^[71]	0	13,800	23,000	–

sets^[37,68] as well as with the all-electron Jorge-TZP-DKH,^[60] Sapporo-DKH-TZP-2012,^[61] and cc-pVTZ-DK^[53] basis sets.

The results suggest that the valence description is very similar at the CASSCF level between the new all-electron SARC basis sets and the ECP-based def2 basis sets. Among the all-electron basis sets, the results obtained with the SARC, the Sapporo, and the correlation-consistent basis sets almost coincide, albeit the partial incorporation of generally contracted functions in the cc-pVTZ-DK basis set may be associated with higher computational cost depending on the integral code employed. On the other hand, the deviating results and inverted order of the two highest orbitals obtained with the Jorge-TZP-DKH basis set are indicative of a deficiency in the description of the d space in its default form. We confirm that this is corrected in the QZP version of the Jorge basis set, which increases the number of d functions by one compared to the TZP version but also extends the high angular momentum functions up to h .

In summary, although the above examples are by necessity limited, they demonstrate that the SARC basis sets perform reliably in typical molecular applications in conjunction with the ZORA and DKH2 Hamiltonians. In comparison to DKH-optimized all-electron basis sets that employ an analogous segmented contraction the SARC are equal or better than existing alternatives, while also offering the option of a ZORA-specific version that can be useful for many types of calculation. Finally, it is noted that since the SARC basis sets are loosely contracted, they retain considerable flexibility in the core region even in their standard form. This can be important for calculations of spectroscopic parameters that depend on a flexible description of the inner-shell electronic structure or the distribution of electronic or spin density close to the nucleus, such as hyperfine couplings, Mössbauer, and X-ray spectroscopy. For the most physically consistent approach to the description of the core region the use of a finite nucleus model should also be considered.

4 | CONCLUSIONS

We presented a series of SARC basis sets for the elements Rb–Xe. The new basis sets extend the SARC family of ZORA- and DKH2-adapted basis sets to cover the 5s, 4d, and 5p block elements. In keeping with their heavier-element congeners, the new basis sets adopt a loose contraction and utilize a common set of exponents for

both Hamiltonians, with the CGTFs optimized separately for each Hamiltonian. Compared to a large reference basis set, the SARC basis sets were shown to perform consistently across the series and are associated with small incompleteness and contraction errors. Calculations of ionization energies and EAs confirmed that the new basis sets perform reliably for atomic properties. Selected molecular examples indicated that the SARC basis sets are robust and either compare very favorably with existing ECP-based and all-electron alternatives or outperform them while offering increased flexibility, and are hence expected to be a reliable choice for practical applications that utilize the DKH2 or ZORA approaches.

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SUPPORTING INFORMATION

Additional supporting information may be found online in the Supporting Information section at the end of this article.

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A2.1 “Making Science Organizations Sustainable – The Mission of the Max Planck Sustainability Network”^[114]



Making Science Organizations Sustainable—The Mission of the Max Planck Sustainability Network

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The Max Planck Sustainability Network (MPSN) is a grassroots network within the Max Planck Society (MPG), with ~370 members from over 60 Max Planck research institutes, aiming to support sustainability within a German science association committed to fundamental research. The MPSN has adopted the twin goals of making research practices within the overall MPG more sustainable and of supporting local Sustainability Groups in making research practices at their individual institutes more sustainable. The MPSN counts members from diverse backgrounds, regarding both academic field of expertise and roles within the MPG. Its activities focus around Energy, Mobility, Supplies and Waste, Biodiversity and Food, with the ambition to assess impact and expense of each proposed measure. The network's long-term vision is to make research more sustainable and to serve as a role model that inspires other scientific organizations to become sustainable and to optimize the operation of research and administration, which require both individual and structural changes.

Keywords: majority vote, Max Planck Society, moral responsibility, research organizations, non-scientific staff, scientific staff, grassroots network, sustainability science

INTRODUCTION

Since its foundation and first general meeting in May 2019, the Max Planck Sustainability Network (MPSN) has attracted over 370 members from over 60 Max Planck Institutes (**Figure 1A**). At over 30 of these institutes, local Sustainability Groups have also formed which are connected through the MPSN. This network aims to support sustainability within the Max Planck Society (MPG)¹, a German science association committed to fundamental research. The MPG holds more than 23,000 affiliated individuals in over 85 institutes, mainly located in Germany but also in Italy, the Netherlands, Luxemburg, and the USA. The MPG supports prominent research on various topics, including climate change, biodiversity, and societal challenges associated with sustainability or the lack thereof. Yet, the MPG currently operates much like most other academic institutions in that

¹ Max Planck Society for the Advancement of Science, German: Max-Planck-Gesellschaft zur Förderung der Wissenschaften e. V.

research is largely conducted without assessing and addressing the ecological consequences of the materials, energy usage, and travel involved in the research process. The work performed in the MPG therefore does not only contribute to the scientific advancement of humankind, but also to anthropogenic emissions of greenhouse gases, waste generation, and depletion of resources. Indeed, if the scientific community has successfully made the first step—acknowledging that humanity is facing an environmental crisis—the second step—acting upon it within our own life and work—is needed. The members of the MPSN feel a moral obligation to address the ecological consequences of their work and to transition toward a more sustainable research environment. Transforming organizations toward more sustainable ones from the employer's perspective has received much interest recently, highlighting the importance of employee engagement (Kim et al., 2016), adapted strategic planning (Batista and Francisco, 2018) and conceptual frameworks to guide invested efforts (Lozano, 2018). The MPSN has therefore adopted the twin goals of making research practices within the overall MPG more sustainable and of supporting local Sustainability Groups in making research practices at their individual institutes more sustainable. The network's long-term vision is to become role models that inspire other scientific organizations to become sustainable and to optimize the operation of research and administration in the MPG toward a system that operates sustainably.

SCIENTISTS' MORAL OBLIGATION

*"Insight must precede application." / "Dem Anwenden muss das Erkennen vorausgehen."
—Max Planck*

The reverse conclusion of Max Planck's quote implies that appropriate application must follow insight. This is especially true for those who have early and direct access to this insight. In the past years and decades, scientists have increasingly urgently called attention to the climate crisis and called for climate action from governments, industry, and citizens. To highlight two examples, over 15,000 scientists signed the "Warning of a climate emergency" (Ripple et al., 2020) and the "Scientists For Future" network is officially supported by 26,000 scientists in German-speaking areas alone (Hagedorn et al., 2019). Addressing the climate crisis and moving toward a sustainable world requires both, research on what is happening and how different problems could be solved, and concrete action and behavior change [see IPCC SR15 report; Rogelj et al. (2018)]—both knowledge and action are indispensable parts of sustainability. Yet, science also produces its share of global greenhouse gas emissions and other negative environmental impacts. On the global level and compared to other emitters such as energy suppliers or food producers, this share is relatively small. However, scientists' carbon footprint per capita is above average (Rosen, 2017; Jean and Wymant, 2019; Langin, 2019; Nature Nanotechnology, 2019). In consequence, many scientists do not only lobby for more climate action in society and politics but are also aiming to reduce their own carbon footprint (Rosen, 2017).

To make research environmentally friendly, scientists need to initiate a process of change management in scientific institutions. Moreover, making research processes more environmentally friendly, scientists' call for global climate action becomes more credible.

Implementing more sustainable practices in research will not be possible without behavioral change and thus limitations which could be perceived as restrictions. For example, the major contribution to the carbon footprint of science presumably is air travel activity (accounting for up to 50% of emissions), especially to conferences (Jean and Wymant, 2019; Langin, 2019; Nature Nanotechnology, 2019; Klöwer et al., 2020). Here, the necessary action is to travel less and especially to fly less.

Such limitations are often criticized for being contradictory to the freedom of science (Vogt and Weber, 2020). Freedom of science refers to the idea that research questions and objectives are formulated by scientists and that the results cannot be influenced or even dictated. However, freedom of science does not imply that scientists can act without any limitations or restrictions. Science has always been and is subject to limitations and restrictions which are imposed by society and politics but also by their own administrations (Beringer and Adomßent, 2008; Bachmann, 2016). On the contrary, by being proactive, science organizations can ensure their own freedom of research. It is probable that society and politics aim to rather increase than decrease legal regulations with regard to aspects of sustainability. Thus, by developing own sustainability strategies, science organizations can either prevent legal regulations or at least contribute shaping them.

Finally, as citizens, scientists have a duty to act for the public good (Douglas, 2009)—because they are in a unique position to access the relevant knowledge, because they have the means to act, and because the credibility of the scientific message regarding the environmental crisis depends on scientists' action upon their own behavior. In consequence, colleagues of the MPG saw a moral obligation to advocate for sustainability in research and founded the Max Planck Sustainability Network for this purpose.

INTERDISCIPLINARITY

Interdisciplinary approaches are crucial in defining and enacting sustainable behaviors within a scientific context. Most importantly, research on sustainability—including climate and environmental research, social science studies on behavioral change, and research on new technologies—paves the way to a sustainable future. The MPSN approaches this goal by exchanging perspectives between multiple scientific disciplines and by assessing the impact of measures both during decision-making and during evaluation. However, beyond these fields with a directly obvious link to sustainability, other fields—even seemingly unrelated ones, such as law, art, or mathematics—provide research and perspectives that are beneficial to developing ideas with which to approach challenges to adopting climate-friendly practices. In the MPSN, the majority

of members currently has a background in traditional natural sciences (Physics, Biology, Chemistry), but individuals from Neuroscience, Psychology, Medical Sciences, or Computer Science are also represented (in total Natural Sciences 85%, Social Sciences 15%; **Figure 1B**). Activities within the network are framed around the existing expertise in the MPG from climate-related research (featured on the MPSN website, invited talks, and seminars on climate topics), but also extend basic research, for example, discussing the psychology of climate beliefs and communication strategies for environmental sciences. Indeed, around one fourth of the scientific staff within the MPSN is currently or planning to do research on sustainability (**Figure 1C**).

Especially as affiliates of a scientific interdisciplinary research organization, MPSN members translate their collective multidisciplinary knowledge into finding solutions to more sustainable research practices. Much like society needs diverse voices to tackle the climate crisis, the MPSN represents all voices from different disciplines and from scientific backgrounds for impactful climate action.

NON-HIERARCHICAL GRASSROOTS ACTION AND INCLUSIVITY

To support sustainability in the MPG and enable interdisciplinary communication, members of the scientific community need to get together and exchange ideas for climate action. Although the support from institutions' leadership and governmental actors is important, climate action will be most effective if members of the scientific community begin organizing, discussing, proposing, and promoting climate action themselves, lobbying executive and legislative powers for changes in rules and regulations rather than passively waiting for such change to happen.

Thus, the MPSN was founded as a grassroots initiative, striving for maximum inclusivity and bottom-up processes and works accordingly by honorary engagement. The MPSN combines local Sustainability Groups from different Max Planck Institutes and a network-wide Steering Committee to foster communication. The statutes of the network are openly available. Official polls and elections are based on a majority judgment grading system (Balinski and Laraki, 2007), which is a recently developed method for finding a compromise in a democratic decisions process. The network is bilingual (German and English, because the network has an internationally diverse membership) and aims to be inclusive (e.g., non-binary, gender-inclusive communication) and non-hierarchical (e.g., through omitting academic titles). Members consider themselves pioneers of a sustainability movement in academia and engage in proposed measures, such as virtual meetings, voluntary self-commitments to fly less, cultivating eco-friendly green spaces at institutes, establishing waste sorting, and open sharing of resources. It is inherently important that both scientific and non-scientific staff are included to turn ideas and concepts into action. Accordingly, the MPSN aims to address all colleagues within the MPG because everyone is a crucial part in finding and implementing

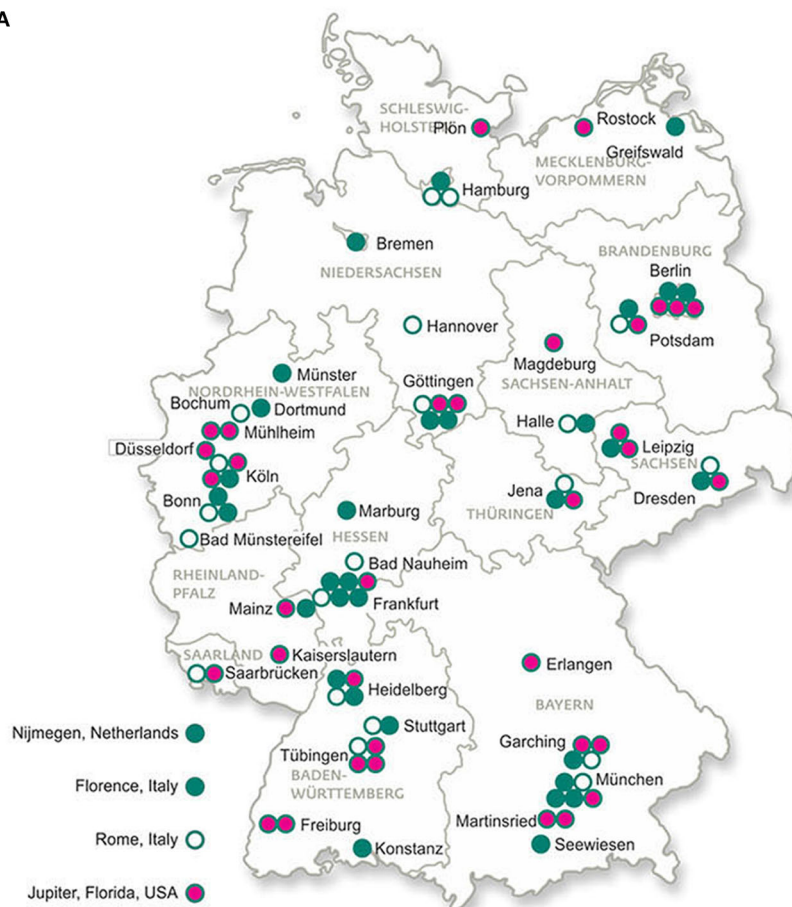
solutions for more sustainability. Scientific and non-scientific staff share the same work environment and the same desire to change the impact of their work regardless of their employee role and are thus on par with each other within the MPSN. Moreover, particular importance is given to the inclusivity of the network, for example, by attempting to represent all levels of staff (technical, scientific, and administrative) in the Steering Committee and in the network itself and by making all events and activities accessible to all members of the network. In the MPG, 9,297 non-scientific colleagues support 14,666 scientists (Max Planck, 2020). The MPSN consists of almost as many scientists (about 53%, referred to as staff whose main task is to publish scientific articles) as non-scientific staff (about 47%, referred to as staff whose main task it to support the scientific staff in their endeavor) (**Figure 1D**).

Similar to how we believe scientific diversity is necessary, we are also convinced that diversity in hierarchy and type of staff is necessary in order to achieve a change toward sustainability within the MPG. Colleagues at different hierarchical levels or positions are confronted with differential environmental aspects or can see different perspectives of the same issue. Within our network we practice a culture of equality, that is, opinions should solely be assessed on the basis of the statement itself and not on the speaker's position of authority.

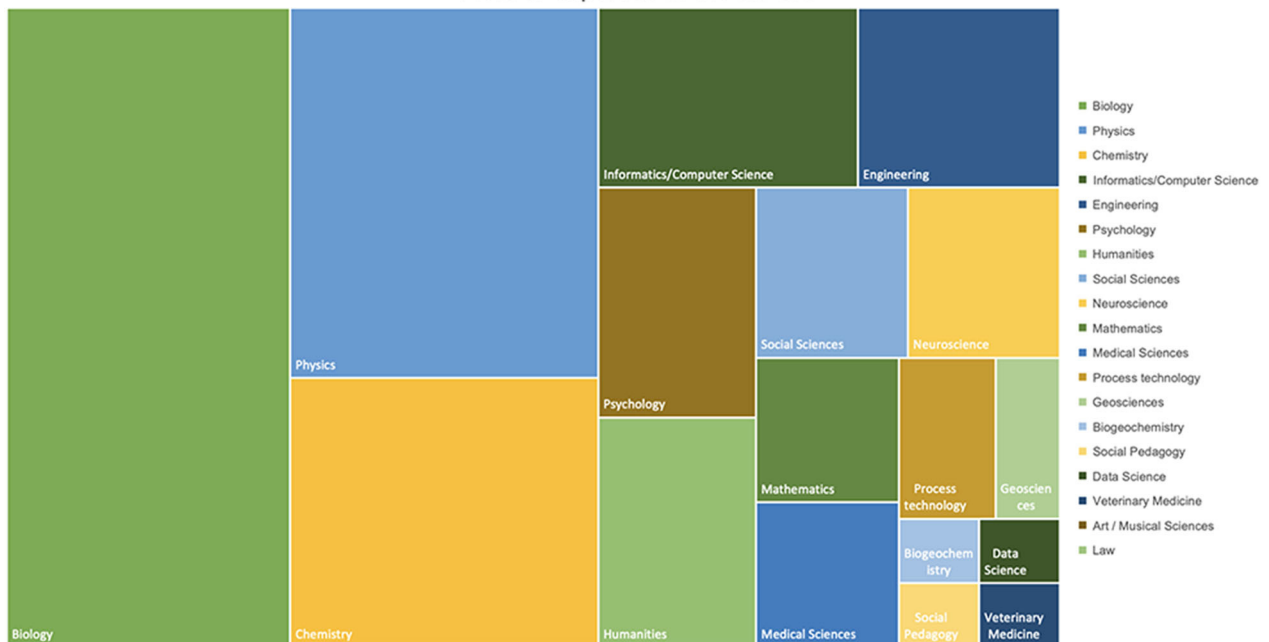
FOCUS OF THE MPSN'S WORK

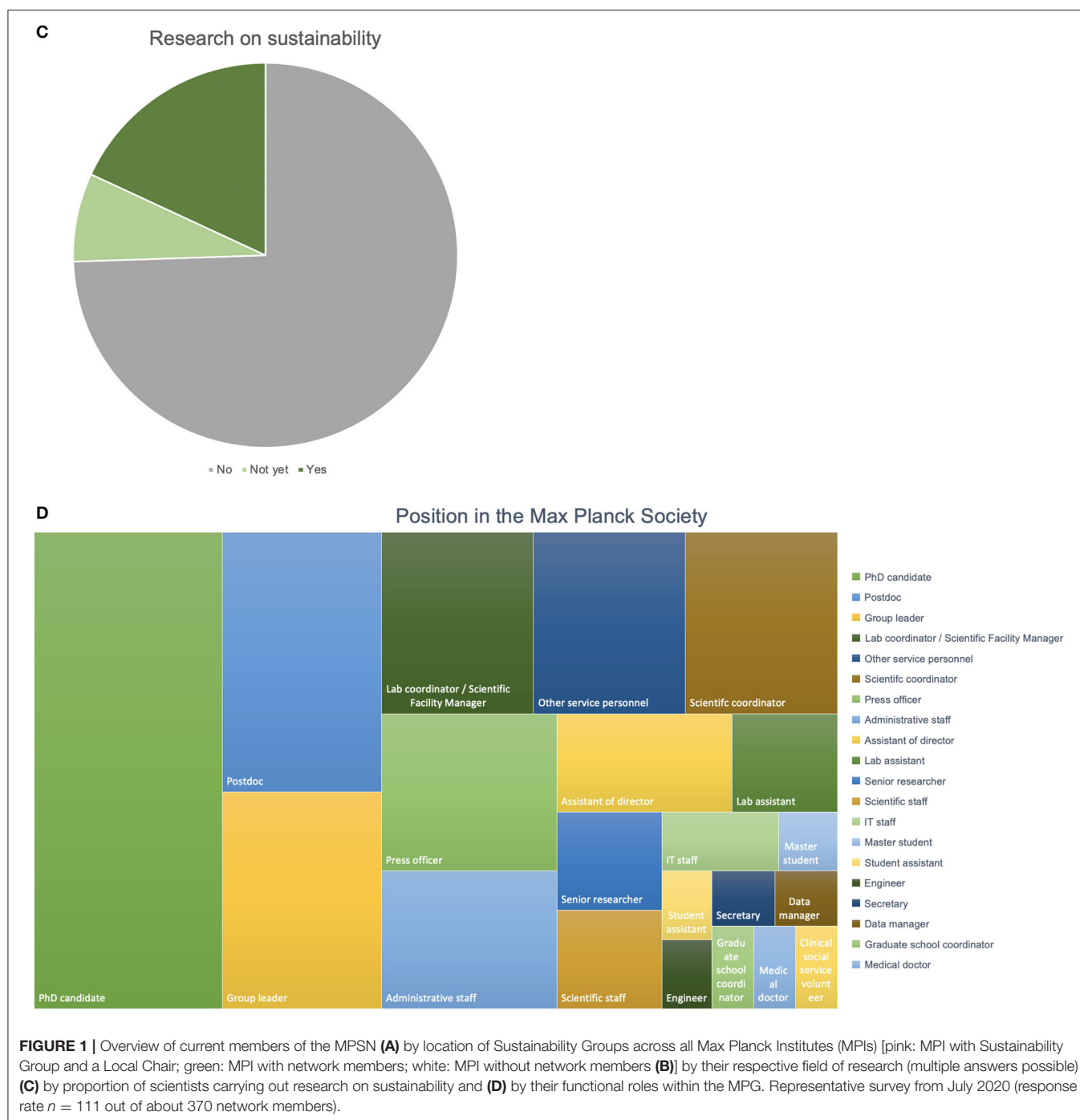
The MPSN aims to compile a catalog of recommendations for the implementation of sustainability measures on the institute level and throughout the MPG. This catalog shall be delivered to the Sustainability Groups and to the president of the MPG. In order to identify firstly the subjectively most important domains covering various aspects of academic and work life, the Steering Committee of the MPSN conducted a survey among its members. The survey included 10 domains and 116 measures rated on importance by 134 members. For the sake of overview and efficiency, the highest rated domains were chosen and similar domains grouped into the five clusters (i) Energy, (ii) Mobility, (iii) Supplies and Waste, (iv) Biodiversity and Food, and (v) Coordination and Assessment (**Figure 2**). Corresponding working groups were formed to create a first version of the catalog of recommendations, outlining and assessing each potential measure according to costs, feasibility, impact, and rating by network.

In addition to the five working groups, MPSN members have already implemented various MPG-wide initiatives pursued by *ad hoc* task forces: Starting off with a MPG-wide voluntary commitment to restrain from short-haul flights (about 480 signatories) and implementing and supporting virtual conferencing tools (Best Practice from the MPSN's Virtual Network Meeting). Further, aiming to influence policy makers, the network authored a position paper on "Compensation of CO₂ Emission Caused by Travel Activity in the Max Planck Society" addressed to the General Administration of the MPG and a proposal for the Reform of the Federal Travel Expenses Act addressed to the German Government.

A**B**

Field of expertise in the MPSN

**FIGURE 1 |** Continued

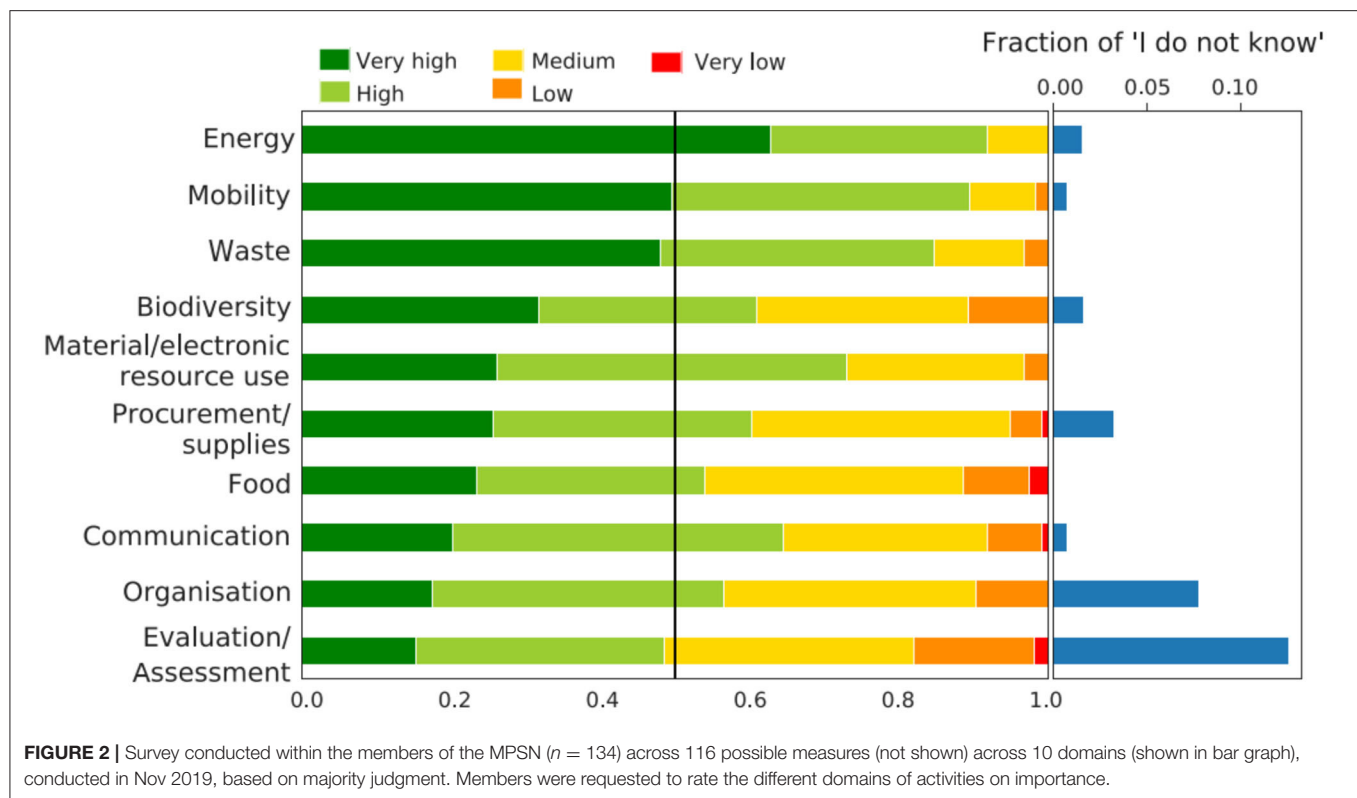


EVALUATING ACTION

The MPSN believes that before taking action, the measures to be implemented need to be carefully assessed. In the decision-making process of implementing sustainable practices, a careful assessment of each measure should be endeavored.

The primary metric for this assessment, is CO₂-equivalent emissions, a metric that is for example useful in assessing the

impact of travel, which much of the MPSN's action has focused on so far. As the network expands and begins addressing other domains such as the footprint of experimental laboratories and the ecological impact of equipment and infrastructure, other proposed metrics such as the multiple indicators used in life-cycle assessments (assessing environmental impacts associated with all the stages of the life-cycle), may become useful to assess diverse ecological impacts. Furthermore, an important first step in the evaluation strategy is to calculate a baseline CO₂



footprint of different institutes (carbon emissions reporting), which the network is currently working on. By repeatedly re-estimating CO₂ footprints over the next years, the MPSN will be able to assess to which extent the implemented measures have reduced emissions.

Beyond the impact of sustainability measures, the network's impact as a whole will be evaluated along multiple dimensions. On the level of the MPSN, an Advisory Board has been formed to counsel and monitor the Steering Committee and thereby ensure that the network's executive meets its internal goals. On the level of the MPG, the aforementioned working groups formulate the internal catalog of recommendations and keep track of which measures have been implemented to which extent. Collectively, the aim of these measures is to track the MPG's progress toward the goals set by the MPSN and to hold the MPSN accountable for its goals, quantifying this progress as much as possible, especially but not exclusively, using CO₂-equivalent emissions as quantitative indicators.

THE MPSN AND OTHER INITIATIVES FOR SUSTAINABILITY IN SCIENCE

Although there are various initiatives across the globe (many of which the MPSN is partnered with), the MPSN stands out in terms of showing all of the following three attributes: being (i) a bottom-up network (ii) within a delimited

national research society and (iii) addressing diverse aspects of sustainability through various organized subgroups. Similar initiatives in other science organizations overlap with some of the above attributes: For example, the employee-driven network EcoInfo within the French National Center for Scientific Research (CNRS) is committed to reduce the environmental impact of data processing at the various CNRS institutions (Montbroussous et al., 2019). The French grassroots initiative Labos1point5, reaches out to more diverse topics of sustainability as an international, inter-organizational network (Cluzel et al., 2020), as do also more top-down organized collectives between independent research institutions, like the University Alliance for Sustainability (Borman et al., 2019) or the International Sustainable Campus Network (Alshuwaikhat et al., 2017). Finally, there exist institutionalized projects to address changes toward sustainable practices within or among research institutions. In Germany, these comprise initiatives like the "Future Campus" at the Forschungszentrum Jülich (Rögner et al., 2017) or the project "Sustainability Management for non-university research institutions" (LeNa) (Daedlow et al., 2016). Through its bottom-up character the MPSN is distinct to the above-mentioned initiatives and to the prevalent employer-focused literature on the topic (Kim et al., 2016; Batista and Francisco, 2018; Lozano, 2018). The MPSN could provide further insight into organizational change management with regard to sustainability from within an organization.

DISCUSSION

Following the official founding (May 2019) and democratic legitimization (statutes released Dec 2019) of the Max Planck Sustainability Network, the MPSN has positioned itself as an important actor within the academic sustainability movement. The network's long-term target is to contribute to the transition of the MPG and its associated institutes toward sustainable organizations and to facilitate this transition through interdisciplinarity, inclusive grassroots action, and through assessment and evaluation. To achieve this target, we investigate and enact measures across different domains (Energy, Mobility, Biodiversity and Food, Supplies and Waste). Some of these measures require behavior change from individual employees, which we will encourage through direct communication and through the participatory nature of our network. However, structural changes are also needed to support and foster such

behaviors, and yet other measures need to be taken on the structural level alone. Taken together, these steps and the MPSN as a whole are aimed toward taking responsibility for the ecological impact of our work and to furthering the role of sustainability and climate action within the scientific community.

DATA AVAILABILITY STATEMENT

The raw data supporting the conclusions of this article will be made available by the authors, without undue reservation.

AUTHOR CONTRIBUTIONS

TF, JM, EM, JHR, JDR, and JS: first draft. MH, SL, EM, and JS: revisions. All authors: contributed to the article and approved the submitted version.

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Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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A2.2 “The “Me too” movement from Hollywood to your bench”^[115]

The #MeToo Movement

BY MAYANK CHUGH, ALBA GONZALEZ
AND JULIAN DAVID ROLFES

from Hollywood to
Our Bench

Sexual harassment is an endemic and dismissive predation that is as prevalent in academia as it is in other fields and workplaces. Certainly, in all cases, dominance and power have made harassment and its concealing properly executable. Women worldwide can surely attest to it. While the stories about assaults are outspoken and highly relatable, the voices against the perpetrators are quiet. Recently, the #MeToo and #TimesUp movements that gained momentum in response to the Harvey Weinstein scandal have encouraged women globally to come together, share their stories and create awareness of sexual harassment – a menace that penetrates cultures and nations. Although these movements and stories are from Hollywood, their roots and messages are not. They are now a testament of sexual misconduct in the workplace. There are many such stories that lie hidden at domestic workplaces and benches across the world. This article is in support of #MeToo, #TimesUp and the other unheard voices to raise awareness of sexual harassment, especially in our offices, labs, and in academia.

#MeToo – Talking about sexual harassment

The #MeToo movement dates back to 2006 when American civil rights activist Tarana Burke used the phrase “#MeToo”, the only thought she could think of, in response to a woman who confessed to being a victim of sexual violence. This phrase was meant to raise awareness of the pervasiveness of sexual abuse and assault in society, and became increasingly famous over time. Eight years later, as a result of previously reported sexual harassment cases inside the film industry, the well-known activist and actress Alyssa Milano unleashed the #MeToo movement on Twitter, encouraging sexual harassment victims to post “MeToo” as part of their status update. #MeToo gave a voice to other well-known actors and actresses, and tens of hundreds of others who have been sexually harassed by their male peers. This triggered a chain of consequences for the offenders, where many were put in quarantine, got fired from their jobs or were formally impeached. The reach and impact of the #MeToo movement went way beyond the red carpet. It has become an international movement, raising awareness of sexual violence around the globe. Moreover, it

highlights the prevalence of sexual violence in certain workplaces, such as the financial, political, military, and academic environments. Women are especially vulnerable in these environments where they face underrepresentation, fierce competition, and where men thrive in the scale of power.

The Weinstein effect and #MeToo have also inspired the birth of the #TimesUp movement from Hollywood celebrities, thus creating more awareness and giving a voice to the women in the entertainment industry and at their workplace.

The #MeTooPhD – Sexual harassment in academia

Academia, as we know it, is a highly hierarchical field. The people in power are the gatekeepers of careers and funding opportunities, and sadly, most of them are men. Academia is just like Hollywood for a variety of reasons. First, men in academia outnumber and shadow women to a very significant level. In the last few years, efforts have been made to promote gender equity in academia with women making it to universities and positions of power; however, it still requires strenuous determination and time to reach even close to equality.

Second, the field of academia is hyper-competitive as there are only a few professional opportunities available compared to the long list of qualified and talented aspirants. Given the cultural diversity and international environments in our offices and research labs, one might imagine that we are way above traditional gender stereotypes and are in an equal and scientific endeavour. We might imagine professors and students going to dinners, conferences, retreats, and getting drinks together. However, this is not the case. Women in academia are still sexually assaulted and harassed by men in power, and due to the tight job market, their voices remain quiet. The ones who choose to speak up are forced to switch jobs entirely, depriving the field of their talent, their passion, and their insights.

In the wake of the #MeToo movement and to show how ubiquitous the problem of sexual harassment is in academia, former tenured professor Dr. Karen Kelsky at the University of Oregon and Illinois Urbana-

Champaign, who now runs an academic job consultancy blog, 'The Professor is in', launched an anonymous survey and #MeTooPhD tag on Twitter in December 2017. The aim of this survey is "Providing a place for women to share stories without fear of censorship or judgement, to know they are not alone, and to find strength in numbers and a foundation from which to recover and perhaps take action", writes Kelsky on her blog. This anonymous survey contrasts law student Raya Sarkar's initiative, which released a list with professors' names who were accused of sexual harassment, promoting the "naming and shaming" tool against sexual abuse.

Kelsky's survey spreadsheet has more than 2000 entries as of April 27th, from over 30 fields of study. The survey shows that most entries are from graduate students, followed by undergraduate students, non-tenured and tenured professors. The stories on this survey share the well-known symptoms of sexual

Timeline of Events

#MeToo is a social media movement with the aim to demonstrate the prevalence of sexual assault and harassment.

2006 – Tatiana Burke first use the phrase "Me Too" to raise awareness of pervasiveness of sexual abuse and assault in society.

Oct 15, 2017 – #MeToo movement started with the actress Alyssa Milano, and went viral in social media.

Until Now – #MeToo movement reached worldwide impact, raising awareness of sexual assault at the working place.

Oct 5, 2017 – Actress Ashley Judd accuses film producer Harvey Weinstein of sexual harassment.

Oct 31, 2017 – Over 80 women had made allegations against Weinstein, the power of this movement was called the "Weinstein effect".

Overview of the events in the #MeToo movement



RAISING AWARENESS

harassment, as Kelsky points out. First, the ubiquity and severity of sexual abuse ranges from glances to proper stalking for months and years to intimidation and rape. Second, there is 'the sheer force of patriarchal solidarity' that protects the assaulters over victims. This, once again, speaks to the power and dominance that rests in patriarchal academia. Third, there is the loss of women from academia. Many women who shared their stories confessed to a change or loss of projects, supervisors, institutions, and/or funding.

These problems are unsurprising to the women in academia. Many women can relate to it and speak about how pernicious the problem of sexual harassment in academia is. In one of the Quartz interviews, Dr. Rebecca Kukla, a Philosophy Professor at Georgetown University, says women have become used to such male behaviour – 'guarding their bodies and keeping things professionally whenever any acts happen. It's a part of job training'. The truth is many women worldwide struggle with anxiety, vulnerability and confusion about the daily misconduct at their workplace, in addition to keeping their families and careers together. The question before us now is: what can we do as a community to safeguard women, to give voices to long-silenced victims and to encourage them to speak up against their assaulters?

From #MeToo to #Oprah

The Max Planck Society (MPS) released an official statement about sexual harassment and sexual violence. Besides a summary of the legal situation in Germany, including the definition of the terms 'sexual assault' and 'sexual violence', the statement also includes a recommendation for disciplinary actions for employers, "ranging from admonition and warning to transfer to a different workstation ... up to dismissal". The employer is also encouraged to take training as part of the disciplinary actions, as well as preventive and clarifying actions. However, the fact that no MPS-wide guidelines exist to this effect makes the appropriateness of the disciplinary action completely dependent on the employer.

Lastly, the possibilities for victims are summarized, i.e.

talking to the internal EO Officer, the MPS Central EO Officer or the Works Council. It's noted that complaints can be made "informally, including verbally or electronically." While the person concerned does not have to be informed until consequences are agreed on, the contact between the victim and the offender should directly be minimized as far as possible. However, we still stand at the same spot. Max Planck Institutes are also quite hierarchical, once again making reporting difficult. This is especially true considering offenders are often the ones who would decide on disciplinary actions. The fact that there is a lack of strict guidelines from the MPS is another impediment to the reporting of such cases.

Although the MPS is aware of the impact and prevalence of sexual violence and has formally created a guideline, more effort should be put towards enforcing specific actions against the offenders irrespective of power and to create an appropriate platform for reporting cases of sexual assault. The Equal Opportunity group at the Max Planck PhNet fights for these rights.

While the institutional and legal actions take their own shapes and ways, we as colleagues, as men, as women and others who we choose to be, should stand in solidarity and support the voices of those who suffer. As Oprah Winfrey put it in her recent Cecil B DeMille win, "When that new day finally dawns, it will be because of a lot of magnificent women, and some pretty phenomenal men fighting hard to make sure that they become the leaders who take us to the time when nobody ever has to say, 'Me too' again."

Further reading

To read the Max Planck Society's statement on sexual harassment and sexual violence, please visit <https://www.mps.mpg.de/5054710/Sexual-harassment-and-sexual-violence.pdf>

Contact of the MPG Central EO Officer: Dr. Ulla Weber (ulla.weber@gv.mpg.de)



Alyssa Milano ✓
@Alyssa_Milano



If you've been sexually harassed or assaulted write 'me too' as a reply to this tweet.

9:21 PM - Oct 15, 2017

♥ 53.4K 💬 92.9K people are talking about this

Original 'Me too' tweet by actress Alyssa Milano

A2.3 “Voluntary Commitment: Climate-Friendly Business Trips – An Overnight Miracle”^[116]

Voluntary Commitment: Climate-Friendly Business Trips – An Overnight Miracle

by Julian D. Rolfes, Evelyn Medawar & Jakob Schweizer

On September 18, 2019, the circulation of a voluntary commitment regarding [climate-friendly business trips](#) started. Its story, however, goes back to May 2019, to the first workshop on “Sustainability in the Max Planck Society” in Magdeburg ([Offspring article](#) covering this workshop and more). At the end of this workshop, an Interim Steering Committee (ISC) was elected with the task to set up a proper and legitimate network structure for the prospective Max Planck Sustainability Network. This was where the voluntary commitment started. The ISC is a bunch of politically well informed, if not actively involved people, with a relation to the MPS and with a heart for Mother Earth. They understand the bigger picture making them a fertile soil to sow the seeds of great friendship.

Evelyn, Jakob and I, are a group that also spends time with each other privately whenever possible. Bridging the distance between Essen, Magdeburg, Berlin and Leipzig, we use a Telegram group to organize ourselves as meetings in person are limited by the geographic distances between us. In this group, we share environment-related information like the Humboldt University’s voluntary commitment for sustainable business travels that got us excited. Without long hesitation, we shared it with the network and initiated the discussion that quickly led to the decision to set up our own voluntary commitment for the MPS. Using the HU’s voluntary commitment as a basis, we set up the MPS version in minutes. After proof-reading by the ISC, we distributed it to the Sustainability Network, PhDnet and Postdocnet. Our voluntary commitment proved to be very successful: Not even a week later, we had 200 signatures! Today, on December 18, we count 436 signatures.

To us, these numbers are immense! We did not even dare to dream about such a resonance, and we hope that the numbers will keep on growing. The response is already a strong message to the members of the MPS to cover the additional costs that typically come with taking the train instead of the plane. The time where money was the only limiting factor is over - and we think it’s time for the MPS to recognize this. We all



Institutes of the MPS which already formed a local Sustainability group.

should recognize our environmental responsibility, and especially as scientists, we should acknowledge that there is no sound reasoning not to – only our ego and our habituation to affordable luxury are holding us back to make the right decisions. I think we should go even further and make the commitment to refrain from short-haul flights an MPS-wide rule; there are several German universities who set a good example already (climatewednesday.org/selbstverpflichtung/ & academicflyingblog.wordpress.com/). To tackle this issue, there are working groups within the Sustainability Network who refine different proposals on CO₂ compensation (to make train rides more sexy and economically interesting) within the MPS and a reformation of the Bundesreisekostengesetz on a federal level.

Currently, having at least one email a day in my inbox from a person who is willing to stay on ground is a huge motivation driver and a nurturing feeling of solidarity to continue working on sustainability within the MPS – and I hope that the inflow of signatures is not going to stop soon. Let all these mindful people continue to bring awareness to the topic of ‘ecological responsibility in business travels’ at their workplaces and may we all – as well as the MPS as a whole – continue the discussion. The Sustainability Network will send a catalogue of proposed measures including the list of signatures for the voluntary commitment to the President of the MPS. I am extremely looking forward to the moment when the network’s proposals and the voluntary commitment arrives at their desk, featuring all the engagement and motivation behind a huge group of scientists caring about sustainability.

If you would like to get involved with the Sustainability Network, look out for your local Sustainability group (if there is none, form one) and sign up to the network’s mailing list at: <https://listserv.gwdg.de/mailman/listinfo/sustainability> – you can also share your story regarding climate-friendly business trips on social media with us via #SciFlyLess.

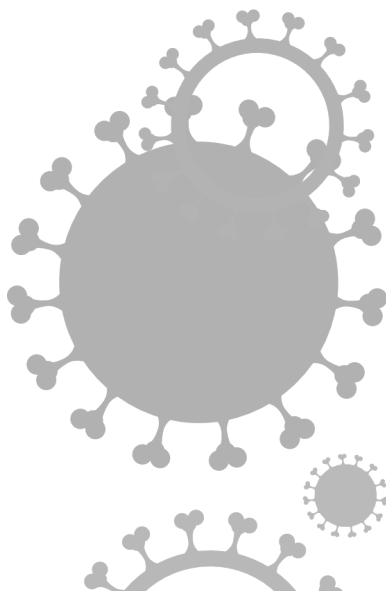


Follow Julian!
@JD_Ro93

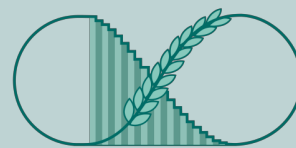


SCAN ME

for an online version of the article



**MAX PLANCK
SUSTAINABILITY NETWORK**



The Max Planck Sustainability network

The Max Planck Sustainability Network (MPSN) is a grassroots network within the Max Planck Society (MPG), with around 370 members from over 60 Max Planck research institutes, aiming to support sustainability within a German science association committed to fundamental research. The MPSN has adopted the twin goals of making research practices within the overall MPG more sustainable and of supporting local Sustainability Groups in making research practices at their individual institutes more sustainable. The MPSN counts members from diverse backgrounds, regarding both academic field of expertise and roles within the MPG. Its activities focus around Energy, Mobility, Supplies and Waste, Biodiversity and Food, with the ambition to assess impact and expense of each proposed measure. The network's long-term vision is to make research more sustainable and to serve as a role model that inspires other scientific organizations to become sustainable and to optimize the operation of research and administration, which require both individual and structural changes.

Read an article by Sustainability Network on Making Science Organizations Sustainable published in *Frontiers in Sustainability*:

SCAN ME

to read the article



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SCAN ME

to visit the Sustainability web-page



A2.4 “Should I stay or should I go (out)?”^[117]

Should I stay or should I go (out)?

by Mental Health Collective of the MPS

Barbara Safaric, Evelyn Medawar, Erica McGale, Olga Vvedenskaya & Julian D. Rolfes



Photo by J. Sessler, Unsplash

Back in 1982, The Clash couldn't help but wonder—

Should I stay or should I go?

Fast forward to 2020, and here we are – amidst a global pandemic, facing the same dilemma. But, is it even a dilemma?

You know how the song continues, don't you?

Should I stay or should I go now?

If I go, there will be trouble

Yes, there will be trouble, as hopefully, many of you are fully aware. The German government recently implemented strict measures in hopes of preventing further spread of COVID-19, emphasizing the importance for people to #stayathome and limit contact with each other to an absolute bare minimum.

Repeat after me: Absolutely. The. Bare. Minimum.

What does this mean to us: Researchers of the Max Planck Society (MPS)?

You are all strongly encouraged to #stayathome. Most institutes of the MPS reduced their operations to a minimum or already closed down with the majority of MPS employees working from home until further notice.

When it comes to regulations within the MPS, make sure to check out the [MAX intranet page](#) that is regularly updated with information relevant to our work.

If you are in a situation where you feel uncomfortable and unsafe to keep coming to work, but your PI still insists on your coming, please write to us at steering.group@phdnet.mpg.de

or steering@postdocnet.mpg.de!

We can keep your identity anonymous, and advocate in your name to the MPS presidential committee.

What about... you know, life?

Are you slowly feeling increasingly anxious, spending all of your time alone or with flatmates/partners? Just like many of us, do you feel the impact of being cut off from your friends, your loved ones and family due to the quarantine, or because they live in different cities and countries all over the planet?

You need to realize, **you are not alone!**

We are all in the same boat, whether it seems like it or not. However, each and every one of us will deal with the current situation in our own way. Everyone has to figure out for themselves what works best for them.

The only thing we can do, and the only thing in this situation that we have complete control over, is ourselves. Please keep this in mind. Stay respectful toward others and have a tiny bit more patience and compassion than you'd have had back in January. Also perhaps, more importantly, have extra patience and compassion for yourself. Be kind to yourself! These are stressful times and we find ourselves in uncharted territory.

So what can we do?

Meeting in person with your loved ones might not be possible for a while, but there are plenty of ways to stay and feel connected, from texting and calling, to skyping and cooking together.

Some things that I personally enjoy are spontaneous virtual coffee dates and "watch parties". Behold my new "night out": a bunch of my friends and I logged into our Zoom accounts and ended up watching the new season of RuPaul's Drag Race together. Not only was this a fun way to interact with people I care about, it was also a very welcome distraction from all the bad news. And of course, it was great to be reminded of RuPaul's age old message "If you don't love yourself, how the hell are you gonna love somebody else!" Also, Netflix recently paired up with Chrome to enable Netflix watch parties through the use of a new Google Chrome extension (check it out here: netflixparty.com).

In addition to "watch parties", your local retailers might offer delivery services now – check them out!

Finally, in times like this, it is more important than ever to give something back to society, if you feel comfortable doing so. One simple but highly effective way you can support your local community is by helping elderly or quarantined people in need: quarantaenehelden.org.



Want to know more?

@mpg_mhc



Can we learn from others who have lived in isolation before?

Quick answer: Yes! There are plenty of people who regularly experience this situation on a daily basis, namely polar explorers, astronauts or sailors. An initiative to help people deal with self-isolation during the outbreak of COVID-19, referred to as #HackCorona on Twitter, provides a great collection of coping strategies and activities such as the ones that can be found on this site: homenauts.com.

Here, we offer you some resources and a few ideas on how to #staysane while being stuck inside your apartment.

EMAP - the Employee and Manager Assistance Program

First and foremost: don't forget about EMAP, the Employee and Manager Assistance Program! EMAP offers a free and immediate consultation by phone or online for all MPS employees and their families.

How does EMAP work?

Call the phone number +49 (0)800 – 38 77 83 6 and indicate that you belong to the MPS.

The foreign number +49 (0)800 – 38 77 83 62 can be reached from the Netherlands, Austria, Switzerland, Italy, Spain and Portugal free of charge.

You can reach the Fürstenberg Institute who is operating EMAP also by email: beratung@fuerstenberg-institut.de. An online consultation is also possible. You can find short instructions at max.mpg.de.

Moreover, the Fürstenberg Institute shared the

following videos on Youtube with information on:

- COVID-19 in German and English
- Organisation of the work in the Home office in German and English
- Work in the Home office with children in German

1. Self-care & exercise

Did you always want to try meditation but you never had the time? The app **Headspace** has a huge collection of guided meditation and other exercises in their current free package – *Weathering the storm*.

There are also other popular apps such as **Calm**, **InsightTimer** and **buddhify**, to name a few, which may be helpful to invest time in your self-care.

With gyms being closed, many of us need to look for new ways to exercise.

Do you have a yoga mat stashed somewhere in the basement? With no other equipment needed – just your body and your breath – these daily virtual yoga classes may be the right thing for you: Engel.Yoga - Munich, Germany.

If a Downward Facing Dog is not really your thing, don't stop there. There are enough Youtube videos as well as plenty of gyms and fitness trainers who are live-streaming their workouts to keep us all motivated and fit. Check out the Facebook pages of your local gym and favorite fitness influencers, and fitness apps for motivation and guided sweat sessions.

Also, you can always go for a walk or a run. Apps like **Nike Run Club**, **Strava** and **Runtastic** will track your speed and distance, give you some tips and guidance. This is also a great way to virtually connect with your friends and keep the spirits high! But please, be responsible! Do it alone, follow your city and state guidelines, and avoid contact with others at all times.

2. Self-improvement

Luckily, we live in the age of the internet and the world is (still) our oyster, at least the virtual one. There are plenty of websites offering multiple courses, many of which are currently for free. Here are our top picks:

- **Udemy**
- **Coursera** (including one of the most popular courses, *The Science of Well-Being*)
- **edX**
- **1,500 Free online courses from Top Universities**

3. Chat

You can join the MPS-wide #corona_social on Rocket.Chat for some uplifting content. Feel free to post positive stuff or content to keep you going during

home office times! You can also find it in the GWDG Rocket.Chat server when you look for #corona_social.

Global Consortium for Academic Mental Health (twitter @GC4AMH) organizes #COVIDCafe several times a week over Zoom. You can meet researchers from around the world to combat social isolation during the pandemic. All the information about these meetings can be found on Twitter handle @GC4AMH. Students, postdoc, staff and faculty are all welcome.

Organize coffee breaks or lunch breaks over Zoom with your lab every other day and try to discuss non-scientific topics. It will help you and your colleagues feel less isolated.

4. Have an urge to help COVID-19-related research?

An initiative has been formed where we can currently "lend our brains" to the people leading the immensely important COVID-19 research efforts. It might be worth signing up, especially if you have some transferable skills, e.g. in data science, crowdfightcovid19.org/volunteers.

So, now you are a few days into your home office. Dishes are washed, laundry is done, you did two morning yoga classes, went for a run, skyped with everyone you could think of...

But now it's raining outside (and you are extra upset about that because you cleaned the windows yesterday!), and honestly, now you need something more low key.

What else can I do? – glad you asked! There's plenty!

Thanks to the virtual oyster, you can enjoy exquisite works of art from around the globe!

Culture & arts*:

**disclosure: This article was initially published in March, 2020, in the middle of the world-wide lockdown due to COVID-19 pandemic. Some sources have been modified (or removed) for this issue of The Offspring Magazine. **

- Royal Opera House London, Wiener Staatsoper, Schaubühne Berlin and NY Metropolitan Opera offered online stream of their events
- Berliner Philharmoniker: www.digitalconcerthall.com
- Free movies of the IDFA (Doc Filmfestival in Amsterdam): www.idfa.nl
- Virtual tours of famous museums: www.travelandleisure.com/attractions/museums-galleries/museums-with-virtual-tours

Nature & cooking:

You can explore wonderful national parks: [5 National Parks You Can Visit Virtually](#)

- Watch nature documentaries:
[Film-Tipps: Naturdokus für die Zeit zuhause](#)
- Or just look at some animals at [African Animals Camera](#) - live video from Africa and [Baby Goat Livestream](#)—baby goat livestream, people!
- You could even brush up on your culinary skills:
[Kitchen Quarantine: Massimo Bottura's Nightly Cookalong on IGTV](#).

Podcasts & audibles

Another amazing way to shut out the outside world for a bit. You can find free audiobooks at [Audible](#).

And something completely different - throw a party for one in your living room! [United We Stream #1: Watergate | ARTE Concert](#) (many more DJs you can find streaming on Facebook and Youtube).

Also, the [Offspring Magazine Podcast](#).

Last, but not least!

Check out all of the resources we put together for Mental Health Awareness Week last year, [especially](#) Immediate Help Document, where you can find specific contacts based on your region.

Still, if you are feeling overwhelmed by everything - **please reach out!** #sharingiscaring

Stay healthy!

Also, just stay at home.

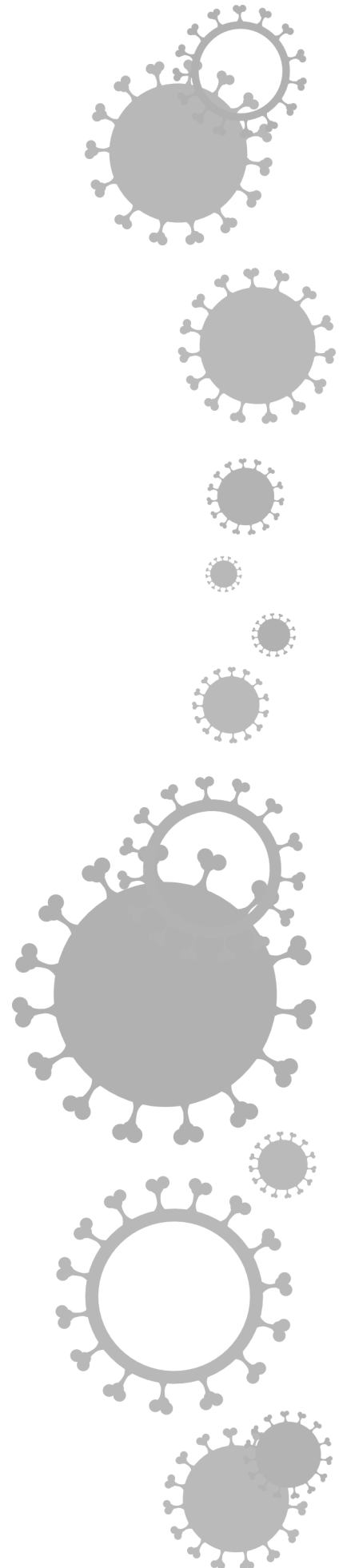


Leonard Nimoy, the original Mr. Spock.
Photo Courtesy: CBS Broadcasting



SCAN ME

for an online version of the article



A2.5 “Black Lives Matter – Black Minds Matter”^[118]

Black Lives Matter - Black Minds Matter

by Mental Health Collective of the MPS

Evelyn Medawar, Olga Vvedenskaya, Julian D. Rolfes & Barbara Safaric

*If you are neutral in moments of injustice,
you have chosen the side of the oppressor.*



[Black Lives Matter protest, Munich, Sat 6 June]

We were casually strolling around New York. Excited, giddy PhDs set free after a conference. We entered a random shop in West Village. The guy at the register sized me up from head to toe, smiled, and said –

“Black is my happy color too.”

Sheepishly returning the smile, I wished the ground would open and swallow me up. I felt incredibly embarrassed. Not because I said something stupid or fell straight on my face. I was ashamed. Of myself. I was wearing a T-shirt with the print “Black is my happy color”. The thought of “black” being connected to anyone’s race and identity did not cross my white privileged mind. How could I be so oblivious? And I like to think I try. That I put an effort into checking in with myself and recognizing how incredibly privileged I am. I should have known better. I have to do better. We all have to do better.

Germany is a racially, ethnically and culturally quite a

diverse country. However, for all their appraisal and celebration of diversity, many institutions lack People of Colour. It is a wide problem that not even the MPS is exempt from. How many People of Color are in your lives? In your lab? At your institute?

Are we suffering from the “out of sight, out of mind” syndrome?

We might. But that does not make our ignorance acceptable. As a part of society, each and every one of us has a responsibility. A responsibility to do good. To do no harm. To help when we can. We all have a part to play.



SCAN ME

for an online version of the article



[Black Lives Matter protest, Leipzig, Sun 7 June]

There is so much to be said, there is so much that needs to be done – what can we do as scientists?

Looking at statistics and numbers (and as scientists, we love data), we rapidly find an overwhelming support for the structural nature of racism: not only do algorithms structurally discriminate against people of color, e.g. when allocating health services¹ or recognizing faces², but also receiving funding³ for research is heavily biased towards white people.

As the research community claims to be generally international, open-minded and diverse, it should stand up and acknowledge existing structural imbalances and the lack of ethnic diversity.

Based on the 2018 Max Planck Society (MPS) annual report⁴, more than 30% of all employees of the MPS were foreign nationals (not German). This number increases to above 50% when looking at scientific employees. Moreover, 37% of institute directors are also non-Germans (112 out of 302). There are no more detailed numbers on ethnicity, but the picture is clear - the MPS community is, in fact, diverse.

Have you ever felt discriminated against?
How will your next scientific home be like?
How do you want it to be like?

As structural problems require structural changes, the first sensible step, we all can and should do, is to acknowledge and become aware of our biases. You might now think “Well, I am not the one with the biases” - please check for yourselves which prejudices you have when it comes to race, religion or gender at [Project Implicit](#).

Acknowledging the status quo, and that we all most likely have some of those implicit or unconscious biases is a good start. Sure, it might be uncomfortable to confront our own biases, but we need to openly discuss these topics and raise awareness, in particular within our research organizations, where **everyone should feel welcomed, independent of their gender, disability, age, sexual orientation and identity, internationality and ethnicity, and religion**. If you are thinking now - “That’s all great, but I’m *just* a doctoral researcher. What impact do I have?” - don’t sell yourselves short, doctoral researchers are more than just another cog in the academic wheel. Change is possible!

But words don’t mean anything unless they are put into action. That’s where we come into play. **Disintegration of systemic racism starts from within ourselves, within our own institutions.**

26th of May is Germany-wide Diversity Day, a campaign of the Charter of Diversity, with the MPS being a member since 2010.

Did you know about it? If you missed the Diversity Day, ask your institute why it wasn’t promoted.

The Code of Conduct of the MPS states:

“We treat each other with respect and do not tolerate any forms of discrimination based on ethnicity, gender, disability, religion or belief, age or sexual orientation or identity. Discrimination has no place in the Max Planck Society: not in the lab, not in the workshop, the office or during the hiring process. We believe that science is a diverse endeavour: diversity provides new impulses, new ideas, new perspectives and innovation.”

Numerous public scientific institution and publishing houses have issued their statements addressing racism in the scientific community, including **Nature**: *Systemic racism: science must listen, learn and change*, **Cell**: *Science has a racism problem*, and **eLife**: *Racism in Science: We need to act now*. On 10th of June, there was a global #ShutDownSTEM day - a call for action to fight racism inside of academia. Thousands of scientists joined world-wide, pointing out the importance of equity.

White privilege is real, there is no point denying it. Have a look at this eye-opening TEDx talk by Dr. Peggy McIntosh, who was the first to write⁴ about white privilege in the late 80's: *How to recognize your white privilege — and use it to fight inequality*.

If you still don't think science has a racism problem, please check out #BlackintheIvory on Twitter and read the countless stories of your fellow scientists describing their experiences with racism they face world-wide. If you are in the mood for some reading (which we heartily recommend), here are a few suggestions to start with: *Superior: the Return of Race Science* by Angela Saini, *Why I'm No Longer Talking to White People About Race* by Reni Eddo-Lodge, *Me and white supremacy* by Layla Saad.

Mental Health Support

Recent events can easily be overwhelming. Black Lives Matter movement has mobilised millions of people all over the planet in the last weeks, with tens of thousands of people joining the protests in Germany as well. Constantly being exposed to reports of incomprehensible violence and injustice the Black community is exposed to, will take a toll on you. Even more so if you are a member of the targeted community.

It is important to take care of yourselves, prioritize your mental health and set boundaries to protect your well-being. We are here to support you in any way we can, from simply talking to you or helping you find a therapist. Please, don't forget about the Employee and Manager Assistance Program (EMAP). If you feel more comfortable contacting us, please don't hesitate and do so. Some of you might have met us by now during **Collective TeaTime**, so you know the faces behind these words.

Therapy has many benefits and there are many factors that will determine how successful it will be. The crucial factor is the relationship that develops between you and the therapists. You need to feel comfortable, relaxed and you need to be able to trust your therapists. Usually you are only asked if you have a preference for female or male therapists. If you are part of the Black community, or any other ethnical minority, it might be easier to open up to a therapist that can understand your cultural background, termed Culturally Sensitive Therapy^{5,6}. The **Black Minds Matter** initiative in the UK raises specific concern for a state of emergency for Black people's well-being by providing culturally trained therapists, support groups and mentorship. Unfortunately, we have failed to find a similar organization in Germany. Official databases of licensed therapists do not include any details beyond the language(s) in which therapy is provided. Also, #ShutDownSTEM compiled an extensive list of resources for Black people who are in the need of healing and self care.

The bottom line - please, check your privilege. Use your privilege to make a change. Educate yourself. Speak up when someone is being harmed. Call out discrimination. Be a decent human being. Be kind. And never forget:

It's not about guilt, it's about responsibility.

References:

¹<https://www.nature.com/articles/d41586-019-03228-6>

²<http://news.mit.edu/2018/study-finds-gender-skin-type-bias-artificial-intelligence-systems-0212>

³<https://www.sciencemag.org/news/2019/10/study-identifies-key-reason-black-scientists-are-less-likely-receive-nih-funding>

⁴White Privilege and Male Privilege: A Personal Account of Coming to See Correspondences Through Work in Women's Studies

⁵Asnaani A, Hofmann SG. Collaboration in multicultural therapy: establishing a strong therapeutic alliance across cultural lines. *J Clin Psychol.* 2012;68(2):187-197. doi:10.1002/jclp.21829

⁶Pakes, K. and Roy-Chowdhury, S. (2007), Culturally sensitive therapy? Examining the practice of cross-cultural family therapy. *Journal of Family Therapy*, 29: 267-283. doi:10.1111/j.1467-6427.2007.00386.x

Being discriminated against should not ever happen.

If you encounter discrimination, need help or support, please contact the Phdnet Equal Opportunity workgroup at equal.opportunity@phdnet.mpg.de or PostdocNet at steering@postdocnet.mpg.de.

Contact points for PhDs in the case of discrimination or conflict

- **Superior**– Your superior is always your first point of contact, when it comes to conflicts within the team, with your peers from your own unit or from other units. If your superior is involved in the conflict, or if you would generally prefer more distance and confidentiality, there are further points of contact that will provide help and advice for finding a solution:
- **Ombudsperson** (at every institute) - Scientific misconduct and problems with supervision. These conversations are treated as confidential.
- **EO Officers** (sometimes still called Gender Equality Officers, at every institute + central EO Officer) - Cases of discrimination/prejudice/harassment
- **Phdnet Steering Group** - Cases for crisis which might involve the general administration for advice on who to contact directly sg@phdnet.de
- **Phdnet EO Workgroup** - Cases of discrimination, lack of EO, or for advice, contact equal.opportunity@phdnet.de
- **Staff Unit "Internal Investigations"**- conducting internal investigations into information on suspected non-scientific misconduct. Dr. Julia Lutz-Seitz, LL.M. Eur.
Phone: +49 89 21 08 26 35
Email: report@mpg.de
- **Law firm** - MPS appointed law firm to help in cases of harassment, mobbing and discrimination: Wirsing Hass Zoller - Rechtsanwälte Partnerschaft MbB, represented as confidants by:

Contact details of Steering group of the

Dr. Christine Dross

Lawyer

Phone: 089 29 00 71-28

Email: dross@wirsing.de

Thomas Müller

Lawyer

Phone: 089 29 00 71-0

Email: t.mueller@wirsing.de

PostdocNet:

steering@postdocnet.mpg.de

www.postdocnet.mpg.de

Equal Opportunity Group of the Phdnet is striving to ensure equity for all doctoral researchers within MPS. Everyone deserves and needs to be treated with respect and presented with the same opportunities, regardless of their age, gender identity or sexual orientation, physical or mental health, race or ethnicity, cultural or social background, external appearance, language, and religion.

Equal Opportunity Group works on solving the problems PhDs encounter along the way towards earning their degree, improving general work conditions and raising awareness in order to fight discrimination and implicit biases.

To achieve equity, numerous barriers on the path towards equal opportunities must be broken down, which is our group's primary goal. In the meantime, we can also help each other by making sure services are available that prop up underrepresented people to overcome those barriers. We also offer information to anyone who encounters a situation of compromised equal opportunities in their institute, with peer-to-peer advice as well as redirection to appropriate people and avenues for action.

Contact details of EO workgroup of the Phdnet:

Equal Opportunity Group of the Phdnet at
equal.opportunity@phdnet.mpg.de

For More Details about the EO WG



A2.6 “Nachhaltigkeits-Netzwerk der Max-Planck-Gesellschaft – Interimsstatuten / Max Planck Sustainability Network – Interim Statutes”

NACHHALTIGKEITS-NETZWERK DER MAX-PLANCK-GESELLSCHAFT – INTERIMS-STATUTEN

PRÄAMBEL

Die Nachhaltigkeitsgruppen der Max-Planck-Institute (MPIs) verfolgen das Ziel, zur Verbesserung der Kommunikation untereinander sowie mit der Gesamtkörperschaft der Max-Planck-Gesellschaft (MPG) ein Nachhaltigkeitsnetzwerk zu etablieren.

1 ZIELE

Die Hauptziele des Netzwerks sind zunächst die Erstellung einer internen Struktur sowie eines Maßnahmenkatalogs.

1.1 STRUKTUR UND ZIELSETZUNGEN

Zur Erarbeitung einer geeigneten internen Netzwerkstruktur haben die auf dem 1. Workshop *Nachhaltigkeit in der MPG* vom 16. bis 17. Mai 2019 am MPI für Dynamik komplexer technischer Systeme in Magdeburg anwesenden Vertretungen der Nachhaltigkeitsgruppen einen Interimssteuerkreis bestimmt und diesen primär mit der Aufgabe betraut, diese Struktur in Zusammenarbeit mit dem Nachhaltigkeitsnetzwerk sowie dem Präsidenten der MPG eine Netzwerkstruktur zu erarbeiten und zu etablieren. Dies beinhaltet die Einführung eines zukünftigen Steuerkreises sowie dessen demokratische Legitimierung. Darüber hinaus verfolgt das Netzwerk die Absicht, die Kommunikation der Nachhaltigkeitsgruppen untereinander zu fördern.

1.2 MAßNAHMENKATALOG

Zur Unterstützung der lokalen Arbeit der Nachhaltigkeitsgruppen arbeitet das Netzwerk an der Aufgabe, einen Maßnahmenkatalog mit konkreten Vorschlägen und Konzepten zur Steigerung der Nachhaltigkeit der MPG zu erstellen.

2 ORGANISATIONSSTRUKTUR

Die derzeitige Struktur des Nachhaltigkeitsnetzwerks besteht aus den lokalen Nachhaltigkeitsgruppen sowie einem Interimssteuerkreis.

2.1 NACHHALTIGKEITSGRUPPEN

Dem in der MPG etablierten hohen Grad an Autonomie der einzelnen MPIs folgend, unterliegt die Organisationsstruktur der lokalen Nachhaltigkeitsgruppen sowie deren Arbeit keinen Einschränkungen, Empfehlungen oder Bestimmungen aus dem Nachhaltigkeitsnetzwerk. Eine Nachhaltigkeitsgruppe ist eine in der Regel formlose Interessensgemeinschaft innerhalb eines oder mehrerer MPIs, die für alle Mitarbeitenden der mit der jeweiligen Nachhaltigkeitsgruppe affilierten MPIs offen steht. Ihr Ziel ist die Praxisoptimierung des eigenen MPIs sowie der gesamten MPG im Sinne der Nachhaltigkeit, unter Berücksichtigung der im Rahmen der MPG notwendigen Freiheit der Grundlagenforschung.

2.2 INTERIMSSTEUERKREIS

Der Interimssteuerkreis ist ein Zusammenschluss aus 10 Personen, welcher auf dem 1. Workshop *Nachhaltigkeit in der MPG* vom 16. bis 17. Mai 2019 am MPI für Dynamik komplexer technischer Systeme in Magdeburg von den anwesenden Vertretungen der Nachhaltigkeitsgruppen einstimmig gewählt wurde. Dabei handelt es sich um folgende Personen in aufsteigender Reihenfolge der Länge ihrer Einträge:

- Martin Vogel (MPI für Biophysik, Frankfurt)
- Harald Rösch (Generalverwaltung, München)
- Christine Gieraths (Generalverwaltung, München)
- Sebastian Hettrich (MPI für Meteorologie, Hamburg)
- Jana Milucka (MPI für Marine Mikrobiologie, Bremen)
- Tanguy Fardet (MPI für biologische Kybernetik, Tübingen)
- Julian Rolfes (MPI für Kohlenforschung, Mülheim an der Ruhr)
- Evelyn Medawar (MPI für Kognitions- und Neurowissenschaften, Leipzig)
- Sophia Pistorius (MPI für Dynamik komplexer technischer Systeme, Magdeburg)
- Jakob Schweizer (MPI für Dynamik komplexer technischer Systeme, Magdeburg)

2.2.1 BESCHLUSSFÄHIGKEIT

Der Interimssteuerkreis verpflichtet sich zu einem Quorum von mindestens fünf Anwesenden. Unabhängig von der Anzahl der Anwesenden benötigt der Interimssteuerkreis eine Mehrheit aus mindestens fünf Stimmen für einen Beschluss.

3 INKRAFTTRETEN

Diese Interims-Statuten treten rückwirkend zum 17. Mai 2019 in Kraft.

Ausgehandelt vom Interimssteuerkreis, 1. Juli 2019.

MAX PLANCK SUSTAINABILITY NETWORK – INTERIM STATUTES

PREAMBLE

The Sustainability Groups of the Max Planck Institutes (MPIs) aim at establishing a Sustainability Network to foster communication among themselves as well as with the body of the Max Planck Society (MPG).

1 AIMS

The initial major aims of the network are to build an internal structure as well as a catalogue of measures.

1.1 STRUCTURE AND OBJECTIVES

At the 1st Workshop *Sustainability in the MPG* from 16th to 17th May 2019 at the MPI for Dynamics of Complex Technical Systems in Magdeburg, the present representatives of the Sustainability Groups elected an Interim Steering Committee. The primary tasks of the Interim Steering Committee are to develop and establish an internal network structure in coaction with the Sustainability Network as well as the president of the MPG. This includes the setup of a future steering committee and its democratic legitimation. The network also aims at fostering communication among the Sustainability Groups.

1.2 CATALOGUE OF MEASURES

To support the local work of the Sustainability Groups, the network works on the development of a catalogue of measures with concrete proposals and concepts to increase the sustainability of the MPG.

2 ORGANIZATIONAL STRUCTURE

The momentary structure of the Sustainability Network consists of the local Sustainability Groups as well as the Interim Steering Committee.

2.1 SUSTAINABILITY GROUPS

Following the high level of autonomy of the MPIs within the MPG, the organizational structure of the local Sustainability Groups as well as their work is not submitted to any restrictions, recommendations or regulations from the Sustainability Network. A Sustainability Group is a generally formless community of interest within one or more MPIs, which is open to all members of the MPIs to which this Sustainability Group is affiliated. Its goal is to optimize practices of the own MPIs as well as the whole MPG in terms of sustainability in consideration of the necessary freedom of fundamental research within the framework of the MPG.

2.2 INTERIM STEERING COMMITTEE

The Interim Steering Committee is a coalition of 10 persons who were elected unanimously by the present representatives of the Sustainability Groups at the 1st Workshop *Sustainability in the MPG*

from 16th to 17th May 2019 at the MPI for Dynamics of Complex Technical Systems in Magdeburg. These 10 persons are, in ascending order of the length of their entries:

- Martin Vogel (MPI for Biophysics, Frankfurt)
- Sebastian Hettrich (MPI for Meteorology, Hamburg)
- Harald Rösch (Administrative Headquarters, Munich)
- Jana Milucka (MPI for Marine Microbiology, Bremen)
- Tanguy Fardet (MPI for Biological Cybernetics, Tübingen)
- Christine Gieraths (Administrative Headquarters, Munich)
- Julian Rolfes (MPI for Coal Research, Mülheim an der Ruhr)
- Evelyn Medawar (MPI for Human Cognitive and Brain Sciences, Leipzig)
- Sophia Pistorius (MPI for Dynamics of Complex Technical Systems, Magdeburg)
- Jakob Schweizer (MPI for Dynamics of Complex Technical Systems, Magdeburg)

2.2.1 QUORUM

The Interim Steering Committee is submitted to a minimum quorum of five attendants. Regardless of the number of attendants, the Interim Steering Committee requires a majority of at least five votes for a decision to be made.

3 ENTRY INTO FORCE

These Interim Statutes enter into force with retroactive effect from 17th May 2019.

Jointly decided by the Interim Steering Committee, 1st July 2019.

A2.7 “Max-Planck-Nachhaltigkeits-Netzwerk – Statuten / Max Planck Sustainability Network – Statutes”

MAX-PLANCK-NACHHALTIGKEITS-NETZWERK – STATUTEN

PRÄAMBEL

Die Nachhaltigkeitsgruppen der Max-Planck-Institute und anderer institutioneller Einrichtungen der Max-Planck-Gesellschaft (in der folgenden Satzung abgekürzt als "MPIs") verfolgen das Ziel, zur Verbesserung der Kommunikation untereinander sowie mit der Gesamtkörperschaft der Max-Planck-Gesellschaft (MPG) ein Nachhaltigkeitsnetzwerk zu etablieren.

§ 1 NAME

Im deutschsprachigen Kontext ist der offizielle Name des Netzwerkes „Max-Planck-Nachhaltigkeitsnetzwerk“. Im englischsprachigen Kontext ist der offizielle Name „Max Planck Sustainability Network“.

§ 2 SPRACHE

Das Netzwerk bemüht sich, zweisprachig zu operieren. Aus Gründen der Praktikabilität sowie der maximalen Inklusion findet die Hauptversammlung (§ 5.2.1) auf Englisch statt. Um die sprachlichen Barrieren so gering wie möglich zu halten, ist das Netzwerk bemüht, besonders auf der Hauptversammlung einfaches Englisch zu benutzen und deutsche Wortmeldungen während der Hauptversammlung explizit zuzulassen und unterstützend zu übersetzen. Als Bezugssprache für diese Statuten wird ebenfalls Englisch gewählt.

Das Netzwerk bemüht sich, nichtbinäre, geschlechterinklusive Sprache zu benutzen. Im Deutschen wird wenn möglich eine neutrale Form (Bsp.: „Das Direktorium sowie alle Mitglieder und Studierende sind zu dem Vortrag eingeladen.“), ansonsten das generische Femininum mit Genderstern (Bsp.: „Unsere Direktor*innen wurden dazu angehalten, jede einzelne Mitarbeiter*in in ihrem Arbeitskreis zu unterrichten.“) und im Englischen das ‚singular they‘ (Bsp.: „Maybe ask your managing director if they are interested in supporting us.“) gewählt.

Das Netzwerk verzichtet auf die Nennung von akademischen Titeln in (unter Anderem) schriftlichen Anreden, Namensschildern und Präsentationen, um den Dialog auf Augenhöhe zu fördern.

§ 3 ZIELE

Die Hauptziele des Netzwerks sind die Optimierung des Forschungs- und Verwaltungsbetriebs in der MPG hin zu einem beispielhafteren und nachhaltigeren Ökosystem sowie die Erleichterung der Kommunikation zwischen den lokalen Nachhaltigkeitsgruppen.

§ 3.1 INTERNE KOMMUNIKATION

Das primäre Hauptziel des Netzwerkes ist die Verbesserung der Kommunikation der Nachhaltigkeitsgruppen (§ 5.1.1) untereinander. Dies soll neben der Hauptversammlung hauptsächlich durch die Arbeit der Arbeitsgruppen (§ 5.2.5) erfolgen.

§ 3.2 EXTERNE KOMMUNIKATION

Das Nachhaltigkeitsnetzwerk basiert auf dem Selbstverständnis der Interessenvertretung innerhalb der MPG. Ziel ist es, die Arbeit und Funktion der MPG im Sinne der Nachhaltigkeit unter Berücksichtigung der von der MPG geforderten Freiheit der Grundlagenforschung zu verbessern.

§ 4 TEILNAHME

Das Nachhaltigkeitsnetzwerk lädt ausdrücklich alle mit der MPG affilierten Personen zur Teilnahme ein. Innerhalb dieser Statuten gelten alle Personen, die eigenständigen Zugang zu den Ressourcen der MPG haben, als mit der MPG affiliert und können am Nachhaltigkeitsnetzwerk teilnehmen, indem sie sich an einer lokalen Nachhaltigkeitsgruppe im Sinne von § 5.1 beteiligen.

§ 5 ORGANISATIONSSTRUKTUR

§ 5.1 LOKALE STRUKTUR

§ 5.1.1 NACHHALTIGKEITSGRUPPEN

Dem in der MPG etablierten hohen Grad an Autonomie der einzelnen MPIs folgend, unterliegt die Organisationsstruktur der lokalen Nachhaltigkeitsgruppen sowie deren Arbeit in Übereinstimmung mit den Netzwerkzielen nur minimalen Anforderungen, um an den Wahlverfahren des Nachhaltigkeitsnetzwerkes teilnehmen zu können. Darüber hinaus unterliegen die Nachhaltigkeitsgruppen keinen Einschränkungen oder Bestimmungen aus dem Nachhaltigkeitsnetzwerk. Eine Nachhaltigkeitsgruppe ist eine Interessensgemeinschaft innerhalb eines oder mehrerer MPIs, die allen mit der MPG affilierten Personen nach § 4 der MPIs, denen diese Nachhaltigkeitsgruppe angehört, offensteht. Ziel ist es, den Forschungs- und Verwaltungsbetrieb der eigenen MPIs sowie der gesamten MPG im Sinne der Nachhaltigkeit unter Berücksichtigung der notwendigen Freiheit der Grundlagenforschung im Rahmen der MPG zu optimieren. Eine neue lokale Nachhaltigkeitsgruppe kann an einem MPI eingerichtet werden, in dem noch keine Gruppe existiert, indem Wahlen gemäß § 5.1.2 durchgeführt und das Wahlergebnis der Arbeitsgruppe "Elections & Research" mitgeteilt wird.

§ 5.1.2 LOKALER VORSTAND

Gemäß § 6.1 wählen die Nachhaltigkeitsgruppen mindestens jährlich (vorzugsweise im ersten Quartal jedes Jahres, nicht jedoch später als drei Monate vor der Hauptversammlung – individuelle Ausnahmen können nach Ermessen des Steuerkreises gewährt werden) einen lokalen Vorstand. Der lokale Vorstand soll aus mindestens einer Person bestehen und nicht mehr Personen als die Zahl der in die jeweilige Nachhaltigkeitsgruppe involvierten MPIs beinhalten.

§ 5.2 ZENTRALE STRUKTUR

§ 5.2.1 HAUPTVERSAMMLUNG

Einmal im Jahr veranstaltet das Nachhaltigkeitsnetzwerk eine Hauptversammlung, zu der zunächst alle lokalen Vorstände und dann alle interessierten Mitglieder der lokalen Nachhaltigkeitsgruppen eingeladen werden. Die Einladung muss mindestens sechs Wochen vor Beginn der Hauptversammlung erfolgen. Hauptziel der Hauptversammlung ist die Festlegung der strategischen Entwicklung des Nachhaltigkeitsnetzwerks und die Vernetzung der Nachhaltigkeitsgruppen untereinander. Ein weiteres Ziel der Hauptversammlung ist die Wissenschaftskommunikation durch Fachvorträge zum Thema Nachhaltigkeit. Die Hauptversammlung wird vom Steuerkreis geleitet.

§ 5.2.2 STEUERKREIS

Jährlich wird nach § 6.2.1 von den Vorständen ein Steuerkreis gewählt, um die Interessen des Nachhaltigkeitsnetzwerks innerhalb der MPG zu vertreten und innerhalb der Netzwerkziele mit Interessengruppen außerhalb der MPG zu nachhaltigkeitsrelevanten Themen zusammenzuarbeiten und zu kommunizieren. Der Steuerkreis ist verantwortlich für die Umsetzung der von der Hauptversammlung verabschiedeten strategischen Entwicklung des Nachhaltigkeitsnetzwerkes. Darüber hinaus ist der Steuerkreis verpflichtet, die lokalen Nachhaltigkeitsgruppen über Fortschritte und Entscheidungen des Nachhaltigkeitsnetzwerkes zu unterrichten sowie die Existenz der in § 5.2.4 genannten ständigen Arbeitsgruppen sicherzustellen.

Der Steuerkreis besteht aus fünf Personen, davon bestenfalls jeweils mindestens einer Person aus den drei Personalgruppen ‚Wissenschaftliches Personal‘, ‚Technisches Personal‘ und ‚Verwaltungspersonal‘. Die Einordnung der Kandidierenden in die Kategorien erfolgt nach eigenem Ermessen vor der Wahl.

Der Steuerkreis wird in seiner Arbeit durch den Beirat und die Arbeitsgruppen unterstützt.

§ 5.2.3 BEIRAT

Der Beirat ist ein vom Nachhaltigkeitsnetzwerk eingesetzter Ausschuss, bestehend aus ehemaligen Steuerkreismitgliedern sowie weiteren Personen und dient der fachlichen Beratung und organisatorischen Unterstützung des Steuerkreises auf Anfrage. Der Beitritt neuer Mitglieder zum Beirat wird von der Hauptversammlung für drei Jahre ratifiziert. Die Auswahl der weiteren Kandidierenden liegt in der Verantwortung des Steuerkreises; die Auswahl, die durch Mehrheitsbeschluss des Steuerkreises erfolgt, muss spätestens mit der Einladung zur Hauptversammlung über die offiziellen Kanäle des Nachhaltigkeitsnetzwerkes veröffentlicht werden und bedarf einer Begründung. Nach Ablauf der drei Jahre endet die Funktion als Mitglied des Beirats, es sei denn, das Mitglied wird von der Hauptversammlung wiedergewählt.

In Einzelfällen kann der Beirat um die vorzeitige Abberufung eines Beiratsmitglieds bitten, dafür benötigt er eine Zweidrittelmehrheit sowie die Zustimmung des Steuerkreises.

§ 5.2.4 ARBEITSGRUPPEN

Die Arbeitsgruppen bilden das Herzstück des Nachhaltigkeitsnetzwerkes. In diesen wird die von der Hauptversammlung festgelegte strategische Entwicklung umgesetzt. Jede Arbeitsgruppe unterliegt einer verantwortlichen Person, die für ein Jahr auf der Hauptversammlung bestimmt wird. Ausnahme bildet die Arbeitsgruppe „Network & Report“, die von dem Steuerkreis geleitet wird. Hierfür kann der Steuerkreis intern ein hauptverantwortliches Mitglied bestimmen. Darüber hinaus dürfen Mitglieder des Steuerkreises sowie des Beirates einer Arbeitsgruppe nur dann vorstehen, wenn keine Person ohne weitere Funktion zur Verfügung steht. Alle mit der MPG affilierten Personen nach § 4 sind

eingeladen, sich in den Arbeitsgruppen zu beteiligen. Alle Arbeitsgruppenleitungen berichten dem Steuerkreis regelmäßig.

Die folgenden vier Arbeitsgruppen werden ständig eingerichtet:

- Arbeitsgruppe „General Meeting“ (Organisation der Hauptversammlung inkl. Einladung der Vortragenden)
- Arbeitsgruppe „Network & Report“ (Verbesserung der Infrastruktur zwischen den Nachhaltigkeitsgruppen und Erstellung eines regelmäßigen Nachhaltigkeitsberichts)
- Arbeitsgruppe „Elections & Research“ (Durchführung der Wahlen sowie Beschäftigung mit Nachhaltigkeitsforschung und Erstellung einer Vorschlagsliste potentieller Vortragender für die Hauptversammlung)
- Arbeitsgruppe „PR“ (Außendarstellung des Nachhaltigkeitsnetzwerks)

Darüber hinaus können weitere Arbeitsgruppen durch den Steuerkreis oder mit Mehrheitsbeschluss des Nachhaltigkeitsnetzwerks eingerichtet werden. Informelle Arbeitsgruppen können jederzeit eingerichtet und im Nachhinein vom Steuerkreis oder mit Mehrheitsbeschluss des Nachhaltigkeitsnetzwerks formell anerkannt werden. Die oben genannten ständigen Arbeitsgruppen können bei Bedarf durch Beschluss der Hauptversammlung in zwei oder mehr Arbeitsgruppen aufgeteilt werden.

§ 5.3 AMTSZEIT

Die Amtszeit der Mitglieder des Beirates, der Arbeitsgruppenleitungen sowie der Vorstände werden nach Einzelfall entschieden. Die Amtszeit des Steuerkreises beginnt in der Regel mit dem 1. Juli und endet mit dem 30. Juni des Folgejahres, aber nicht, bevor eine Nachfolge gewählt wurde.

Sollte ein Mitglied des Steuerkreises vor Beendigung der Amtszeit aus dem Amt scheiden, so führt die Arbeitsgruppe "Elections & Research" dem allgemeinen Verfahren nach § 6.2.1 folgend eine Wahl zur Bestimmung der Nachfolge durch. Dies soll innerhalb eines Monats nach Ausscheiden der Vorgänger*in erfolgen und über die offiziellen Kanäle des Nachhaltigkeitsnetzwerks bekanntgegeben werden. Sollte ein Mitglied des Steuerkreises während der Amtszeit den Status als mit der MPG affilierte Person nach § 4 verlieren, wird der Steuerkreis vor dem eventuellen Ausscheiden der betroffenen Person versuchen, über den Einzelfall zu entscheiden. Das Ausscheiden eines Vorstandes einer Nachhaltigkeitsgruppe sowie einer Arbeitsgruppenleitung ist mit Neuwahlen in den jeweiligen Nachhaltigkeits- oder Arbeitsgruppen zu kompensieren.

Alle gewählten Mitglieder des Nachhaltigkeitsnetzwerks verpflichten sich zu einem angemessenen Wissenstransfer an ihre Nachfolger*innen. Der ausscheidende Steuerkreis schult den neugewählten Steuerkreis vom Moment der Wahl bis zum Amtswechsel. Mindestens ein Mitglied des ausscheidenden Steuerkreises soll nach § 6.2.2 in den Beirat aufgenommen werden.

§ 6 WAHLEN UND ABSTIMMUNGEN

Innerhalb des Nachhaltigkeitsnetzwerkes gibt es verschiedene Formen der Wahlen für verschiedene Positionen.

§ 6.1 LOKAL: WAHL DES VORSTANDS

Das Nachhaltigkeitsnetzwerk interpretiert sich selbst als Graswurzelnetzwerk. Dem in der MPG etablierten hohen Grad an Autonomie der einzelnen MPIs folgend sind die zentralen Vorgaben für die Durchführung der lokalen Arbeit oder der Wahl des Vorstands so gering wie möglich gehalten mit der Intention, die demokratische Legitimierung des Netzwerkes sicherzustellen. Die einzigen Vorgaben sind die lückenlose Dokumentation sowie die Kommunikation des Wahlergebnisses an den Steuerkreis oder die Arbeitsgruppe „Elections & Research“.

Bei begründeten Unstimmigkeiten behält sich der Steuerkreis vor, eine Wahl zu annullieren. Eine Praxisempfehlung für die Wahl des Vorstands ist in Anhang 1 zusammengefasst.

§ 6.2 ZENTRAL: WAHLEN UND ABSTIMMUNGEN AUF NETZWERKEBENE

Die Wahlen auf zentraler Ebene des Nachhaltigkeitsnetzwerkes umfassen vor allem die Wahlen der zentralen Ämter sowie die Ratifizierung von Änderungen in diesen Statuten. Folgende Wahlen werden von den Vorständen der lokalen Nachhaltigkeitsgruppen durchgeführt und erfolgen grundsätzlich anonym und elektronisch unter der Einhaltung der gesetzlichen Datenschutzbestimmungen sowie der Datenschutzbestimmungen der MPG. Basierend auf der generellen Struktur des Netzwerkes sowie der gesamten MPG, erhält jedes MPI eine Wahlstimme. Vorstände, die mehr als ein MPI vertreten, erhalten die Anzahl an Stimmen entsprechend der Anzahl an von ihnen repräsentierten MPI's.

§ 6.2.1 WAHL DES STEUERKREISES

Der Steuerkreis wird nach § 5.2.2 einmal im Jahr gewählt. Die Wahl soll auf der Hauptversammlung stattfinden. Dabei wird als Wahlsystem eine Adaption des „Majority Judgement“¹ festgelegt:

Kandidieren können alle mit der MPG affilierten Personen nach § 4. Die Kandidierenden für den Steuerkreis ordnen sich vor der Wahl nach eigenem Ermessen in eine der drei Personalkategorien ein:

- Wissenschaftliches Personal
- Technisches Personal
- Verwaltungspersonal

Um jede der drei Kategorien abzudecken, ist zu jeder Personalkategorie mindestens eine Kandidatur wünschenswert. Die Kandidierenden können ihre Kandidatur begründen; akademische Titel und berufliche Stellung innerhalb der MPG über die genannten Kategorien hinaus sollen dabei nicht genannt werden. Eine grobe Verletzung kann nach Ermessen des amtierenden Steuerkreises zum Ausschluss von der Wahl führen.

Anschließend können alle Vorstände ihre Meinung zu allen Kandidierenden äußern, indem sie ihnen keine (Enthaltung) oder eine der folgenden Aussagen zuweisen:

- Exzellent
- Gut
- Tolerierbar
- Unzureichend
- Inakzeptabel (Ablehnung)

Um sicherzustellen, dass alle Personalkategorien durch mindestens eine Person vertreten sind, werden die drei Kandidierenden mit der besten Medianen in jeder Kategorie sowie die beiden

¹ PNAS **2007**, 104 (21), 8720–8725. DOI: 10.1073/pnas.0702634104

Kandidierenden mit den besten verbleibenden Medianen in allen Kategorien ausgewählt. Diese fünf gewählten Mitglieder bilden den neuen Steuerkreis. Wenn zwei oder mehr Kandidierende die gleichen Mediane aufweisen, werden die Medianwerte nach und nach von Kandidierenden mit den gleichen Medianwerten entfernt, bis die Medianwerte unterschiedlich werden und somit zu einer Entscheidung führen.

Die Wahl wird durch die Arbeitsgruppe „Elections & Research“ in enger Abstimmung mit dem amtierenden Steuerkreis durchgeführt. Die Wahlergebnisse sind der Öffentlichkeit zugänglich zu machen. Erfolgt die Wahl nicht auf der Hauptversammlung, ist der amtierende Steuerkreis in enger Abstimmung mit der Arbeitsgruppe „Elections & Research“ verpflichtet, den genauen Ablauf der Wahl auf der Hauptversammlung vorzustellen und über eine informelle Abstimmung nach § 6.3.1 von der Hauptversammlung ratifizieren zu lassen.

§ 6.2.2 WAHL DES BEIRATS

Die Beiratswahlen werden nach der Wahl des neuen Steuerkreises durchgeführt. Es gibt drei Arten von Kandidierenden, die für jeweils drei Jahre in den Beirat berufen werden können:

1. Ordentliche Kandidatur: Die Mitglieder des scheidenden Steuerkreises, die nicht wiedergewählt wurden, können sich zur Wahl in den Beirat aufstellen lassen.
2. Außerordentliche Kandidatur: Wie in § 5.2.3 beschrieben, kann der amtierende Steuerkreis weitere Personen für eine außerordentliche Aufnahme in den Beirat vorschlagen.
3. Wiederwahl: Nach Ablauf der drei Jahre können Mitglieder des Beirates wiedergewählt werden. Es gibt keine Beschränkungen, wie oft eine Person wiedergewählt werden kann.

Die Vorstände können ihre Stimme zu den Kandidierenden in folgenden Kategorien abgeben:

- Dafür
- Enthaltung
- Dagegen

Um in den Beirat aufgenommen zu werden, müssen für die Kandidat*in zwei Bedingungen erfüllt sein:

1. Mehr als 25% stimmen für den Beitritt (das erste Quartil ist „Dafür“)
2. Weniger als 25% stimmen gegen den Beitritt (das dritte Quartil ist nicht „Dagegen“)

Sind beide Bedingungen erfüllt, wird die Kandidat*in für die Dauer von drei Jahren in den Beirat aufgenommen. Wenn eine oder mehrere der Bedingungen nicht erfüllt sind, wird die Kandidat*in nicht zugelassen.

§ 6.2.3 RATIFIZIERUNG NEUER STATUTEN

Der Steuerkreis kann Änderungsanträge für diese Statuten erstellen. Die Änderungsvorschläge müssen den Vorständen mindestens zwei Wochen vor dem Beginn der Hauptversammlung mitgeteilt werden. Auf der Hauptversammlung müssen die Änderungen besprochen werden. Dort können die Vorschläge auf Antrag einer auf der Hauptversammlung anwesenden Person durch informelle Abstimmungen nach § 6.3.1 abgeändert werden. Um die Änderungen anzunehmen, bedarf es einer Zweidrittelmehrheit der abstimmberechtigten Vorstände.

§ 6.2.4 WAHLVERTRETUNG DES VORSTANDS

Sollte ein Vorstandsmitglied für die Hauptversammlung verhindert sein, kann das Stimmrecht durch eine schriftliche Vollmacht auf eine Vertretung übertragen werden. Jeder auf der Hauptversammlung anwesende Vorstand ist neben dem eigenen Stimmrecht mit höchstens einem weiteren übertragenen Stimmrecht stimmberechtigt.

§ 6.3 INFORMELLE ABSTIMMUNGEN UND WAHLEN

Die informellen Abstimmungen bestehen aus den Abstimmungen über die von der Hauptversammlung vorgeschlagenen Anträge sowie aus der Wahl der Arbeitskreisleitungen. Alle Mitglieder der Hauptversammlung sind zur Teilnahme an den informellen Abstimmungen berechtigt. Die informellen Abstimmungen können verbal oder per Handzeichen durchgeführt werden.

§ 6.3.1 ABSTIMMUNGEN ÜBER ANTRÄGE

Nach Ermessen des Steuerkreises kann über einen von einem Mitglied der Hauptversammlung eingebrachten Antrag sofort eine informelle Abstimmung durchgeführt werden. Ein erfolgreicher Antrag bedarf der einfachen Mehrheit der Stimmen aller anwesenden Mitglieder der Generalversammlung; in diesem Fall muss der Antrag angenommen werden. Ein Antrag darf nicht dazu verwendet werden, größere Abstimmungen zu umgehen.

§ 6.3.2 WAHL DER ARBEITSKREISLEITUNG

Mit Ausnahme der Arbeitsgruppe „Network & Report“ führen die Mitglieder jeder Arbeitsgruppe eine informelle Abstimmung durch, um die Leitung dieser Gruppe zu wählen. Jede Wahl erfordert eine einfache Mehrheit der Stimmen der Mitglieder der Gruppe. Mit der Übermittlung des Ergebnisses an den Steuerkreis erlangt es Gültigkeit.

§ 7 INKRAFTTRETEN

Diese Statuten treten am Tag nach ihrer Veröffentlichung über die Kommunikationskanäle des Nachhaltigkeitsnetzwerks in Kraft, nachdem sie mit dem Nachhaltigkeitsnetzwerk diskutiert und von der Mehrheit der Mitglieder des Interimssteuerkreises genehmigt wurden.

Ausgehandelt vom Interimssteuerkreis, 17. Dezember 2019.

Geändert durch die 1. Hauptversammlung, 28. Mai 2020.

ANHANG 1 – WAHL DES VORSTANDS – PRAXISVORSCHLAG

Die Wahl zum Vorstand einer lokalen Nachhaltigkeitsgruppe sollte allen mit der MPG affilierten Personen nach § 4 – mit der Einschränkung der Affiliierung zu den an der Nachhaltigkeitsgruppe beteiligten MPis – freistehen. Entsprechend sollte der Aufruf zur Kandidatur mit Bekanntgabe des Zeitpunktes und des Ortes der Wahl sowie einem Kontakt der Wahlleitung mindestens zwei Wochen vor der Wahl schriftlich für alle an den an der Wahl beteiligten MPis affilierten Personen öffentlich zugänglich erfolgen. Dies kann über einen Aushang an einem zentralen Ort oder eine Rundmail geschehen. Die Kandidatur sollte für einen Zeitraum von mindestens drei Werktagen möglich sein.

Die Wahl kann auf elektronischem oder analogem Wege erfolgen. In jedem Fall sollte die Wahl anonym durchgeführt werden. Die gesetzlichen und MPG-internen Datenschutzbestimmungen sind einzuhalten. Bei Bedarf zur Unterstützung kann der Steuerkreis oder die Arbeitsgruppe „Elections & Research“ kontaktiert werden.

Mitarbeitende, die mit mehreren MPIs affiliert sind, sollten vor der Wahl entscheiden, an welchem MPI sie wahlberechtigt sein möchten. Die Wahl der Vertretungen verschiedener MPIs können im gleichen Wahlgang erfolgen.

Die Wahl sollte von einem Komitee vorbereitet und durchgeführt werden, welches aus mindestens zwei Personen besteht, die selbst nicht zur Wahl in den Vorstand kandidieren. Das Komitee hat den Auftrag, die Rechtmäßigkeit sowie die Dokumentation der Wahl sicherzustellen und die Ergebnisse an die Arbeitsgruppe „Elections & Research“ weiterzuleiten. Die Ergebnisse sollten folgende Daten enthalten:

- Namen des Wahlkomitees
- Name(n) des neu gewählten Vorstands
- Versicherung der Rechtmäßigkeit der Wahl durch das Wahlkomitee
- Amtsantritt des neu gewählten Vorstands (Amtsdauer: 1 Kalenderjahr ab Annahme der Wahl)
- Annahme der Wahl durch den neu gewählten Vorstand

Sollte ein Vorstandsmitglied vorzeitig aus dem Amt scheiden, soll eine neue Wahl veranlasst werden. Dies ist auch der Fall, wenn ein Vorstandsmitglied den Affiliertenstatus nach § 4 verliert oder das vertretene MPI für mehr als 4 Monate verlässt.

MAX PLANCK SUSTAINABILITY NETWORK — STATUTES

PREAMBLE

The Sustainability Groups of the Max Planck Institutes and other institutional entities of the Max Planck Society (in the following statutes abbreviated as ‘MPIs’) aim at establishing a Sustainability Network to foster communication among themselves as well as with the body of the Max Planck Society (MPG).

§ 1 NAME

In German context the official name of the network is “Max-Planck-Nachhaltigkeitsnetzwerk”. In English context the official name is “Max Planck Sustainability Network”.

§ 2 LANGUAGE

The network strives to operate bilingually. For reasons of practicality and maximal inclusion, the General Meeting (§ 5.2.1) will be held in English. In order to keep language barriers as low as possible, the network endeavours to use simple English, especially at the General Meeting, and to explicitly allow and support the translation of German contributions during the General Meeting. English is also chosen as the reference language for these statutes.

The network endeavours to use non-binary, gender-inclusive language. In German a neutral form is chosen if possible (e.g.: “Das Direktorium sowie alle Mitglieder und Studierende sind zu dem Vortrag eingeladen.”), otherwise the generic feminine with gender asterisk (e.g.: “Unsere Direktor*innen wurden dazu angehalten, jede einzelne Mitarbeiter*in in ihrem Arbeitskreis zu unterrichten.”), and in English the ‘singular they’ (e.g.: “Maybe ask your managing director if they are interested in supporting us.”).

The network omits to mention academic titles in (among other things) written salutations, name tags and presentations in order to promote dialogue at eye level.

§ 3 OBJECTIVES

The main objectives of the network are to optimize the operation of research and administration in the MPG towards a more exemplary and sustainable ecosystem as well as facilitate communication among local Sustainability Groups.

§ 3.1 INTERNAL COMMUNICATION

The primary objective of the network is to improve communication between Sustainability Groups (§ 5.1.1). Apart from the General Meeting, this is to be achieved mainly through the work of the Working Groups (§ 5.2.5).

§ 3.2 EXTERNAL COMMUNICATION

The Sustainability Network is based on the self-conception of the representation of interests within the MPG. Its goal is to improve the work and function of the MPG in terms of sustainability while taking into account the freedom of basic research required by the MPG.

§ 4 PARTICIPATION

The Sustainability Network explicitly invites all MPG-affiliated individuals to participate. Within these statutes, all persons who have autonomous access to MPG resources are regarded as MPG-affiliated and can take part in the Sustainability Network by participating in a local Sustainability Group as defined in § 5.1.

§ 5 ORGANIZATIONAL STRUCTURE

§ 5.1 LOCAL STRUCTURE

§ 5.1.1 SUSTAINABILITY GROUPS

Following the high level of autonomy of the MPIs within the MPG, the organizational structure of the local Sustainability Groups as well as their work in accordance with the network goals is only subjected to minimal requirements in order to participate in the election procedures of the Sustainability Network. Apart from that, Sustainability Groups are not submitted to any restrictions or regulations from the Sustainability Network. A Sustainability Group is a general community of interest within one or more MPIs, which is open to all MPG-affiliated individuals as defined in § 4 of the MPIs to which this Sustainability Group is affiliated. Its goal is to optimize the operation of research and administration of its own MPIs as well as the whole MPG in terms of sustainability in consideration of the necessary freedom of fundamental research within the framework of the MPG. A new local Sustainability Group can be established at an MPI where no group is yet existing by holding elections according to § 5.1.2 and communicating the election result to the “Elections & Research” Working Group.

§ 5.1.2 LOCAL CHAIR

Following § 6.1, the Sustainability Groups host an election of a Local Chair at least annually (preferably in the first quarter of each year, but not later than three months before the General Meeting – individual exceptions can be granted at the discretion of the Steering Committee). The Local Chair should consist of at least one person and should not contain more persons than the number of MPIs involved in the respective Sustainability Group.

§ 5.2 CENTRAL STRUCTURE

§ 5.2.1 GENERAL MEETING

Once a year, the Sustainability Network organises a General Meeting to which initially all Local Chairs and then all interested members of the local Sustainability Groups are invited. The invitation must be sent out at least six weeks before the start of the General Meeting. The main objective of the General Meeting is to determine the strategic development of the Sustainability Network and to link the

Sustainability Groups together. A further goal of the General Meeting is science communication through lectures from experts on the subject of sustainability. The General Meeting will be chaired by the Steering Committee.

§ 5.2.2 STEERING COMMITTEE

A Steering Committee is elected annually by the Local Chairs in accordance with § 6.2.1 in order to represent the interests of the Sustainability Network within the MPG and, within the network goals, to collaborate and communicate with stakeholders outside of MPG in sustainability-relevant topics. The Steering Committee is responsible for implementing the strategic development of the Sustainability Network approved by the General Meeting. In addition, the Steering Committee is obliged to inform the local Sustainability Groups about progress and decisions of the Sustainability Network as well as to ensure the existence of the permanent Working Groups mentioned in § 5.2.4.

The Steering Committee consists of five persons, with at best at least one person from each of the three personnel groups 'Scientific Personnel', 'Technical Personnel' and 'Administrative Personnel'. The classification of the candidates into the categories takes place at their own discretion before the election.

The Steering Committee is supported in its work by the Advisory Board and the Working Groups.

§ 5.2.3 ADVISORY BOARD

The Advisory Board is a committee set up by the Sustainability Network, consisting of former members of the Steering Committee as well as additional individuals and provides technical advice and organisational support for the Steering Committee on request. The accession of new members to the Advisory Board is ratified by the General Meeting for a period of three years. The selection of additional candidates is the responsibility of the Steering Committee; this selection, ratified by a majority vote of the Steering Committee, must be published via the official channels of the Sustainability Network at the latest with the invitation to the General Meeting and requires a justification. After three years, the function as member of the Advisory Board ends unless the member is being re-elected by the General Meeting.

In individual cases, the Advisory Board may request the early removal of an Advisory Board member, for which it requires a two-third majority and the approval of the Steering Committee.

§ 5.2.4 WORKING GROUPS

The Working Groups form the heart of the Sustainability Network. They implement the strategic development defined by the General Meeting. Each Working Group is subject to a responsible person who is appointed for one year at the Annual General Meeting. Only exception is the "Network & Report" Working Group, which is headed by the Steering Committee. For this, the Steering Committee may internally appoint a Chief Executive Member. In addition, members of the Steering Committee as well as the Advisory Board may only chair a Working Group if no person without a further function is available. All MPG-affiliated individuals as defined in § 4 are invited to participate in the Working Groups. All Working Group leaders report regularly to the Steering Committee.

The following four Working Groups will be established on a permanent basis:

- Working Group "General Meeting" (Organization of the General Meeting incl. invitation of the speakers)

- Working Group “Network & Report” (Improvement of the infrastructure between the Sustainability Groups and preparation of a regular Sustainability Report)
- Working Group “Elections & Research” (Execution of the elections, engagement with sustainability research, and preparation of a proposal list of potential speakers for the General Meeting)
- Working Group „PR“ (Public image of the Sustainability Network)

In addition, further Working Groups may be set up by the Steering Committee or by majority vote from the Sustainability Network. Informal Working Groups can be set up anytime and be formally acknowledged in retrospect by the Steering Committee or by majority vote from the Sustainability Network. The permanent Working Groups referred to above may be divided into two or more Working Groups by decision of the General Meeting if necessary.

§ 5.3 TERMS OF OFFICE

The terms of office of the members of the Advisory Board, the Working Group leaders, and the Local Chairs are decided on an individual basis. The term of office of the Steering Committee usually begins on 1 July and ends on 30 June of the following year, but not before a successor has been elected.

If a member of the Steering Committee leaves office before the end of their term of office, the Working Group “Elections & Research” will cast an online vote following the general procedure of § 6.2.1 to determine the successor. This shall take place within one month of the departure of the predecessor and shall be announced through the official channels of the Sustainability Network. Should a member of the Steering Committee lose the status as MPG-affiliated individual as defined in § 4 during their term of office, the Steering Committee will attempt to decide on the individual case before the resignation of the affected person. The resignation of a local Chair or a Working Group leader must also be compensated for by new elections to the respective Sustainability or Working Groups.

All elected members of the Sustainability Network commit themselves to an appropriate transfer of knowledge to their successors. The outgoing Steering Committee trains the newly elected Steering Committee from the moment of election until the change of office. At least one member of the retiring Steering Committee shall be admitted to the Advisory Board in accordance with § 6.2.2.

§ 6 ELECTIONS AND VOTES

Within the Sustainability Network there are different forms of elections for different positions.

§ 6.1 LOCAL: ELECTION OF LOCAL CHAIRS

The Sustainability Network interprets itself as a grassroots network. In line with the high degree of autonomy of the individual MPIs established within the MPG, the central guidelines for the implementation of the local work or the election of the Local Chairs are kept as low as possible within the goals of the network with the intention of ensuring the democratic legitimacy of the network. The only requirements are the seamless documentation and communication of the election results to the “Elections & Research” Working Group.

In the event of justified discrepancies, the Steering Committee reserves the right to cancel an election. A best practice recommendation for the election of the Local Chairs is summarized in Appendix 1.

§ 6.2 CENTRAL : ELECTIONS AND VOTES ON NETWORK LEVEL

Elections at the central level of the Sustainability Network mainly include elections to central offices and ratification of amendments to these Statutes. The following elections are conducted by the Local Chairs of the local Sustainability Groups and are conducted anonymously and electronically in compliance with the legal data protection provisions as well as the data protection provisions of the MPG. Based on the overall structure of the Network as well as the whole MPG, each MPI holds one voting right. Hence, Chairs representing more than one MPI have a number of votes equal to the number of MPI's they represent.

§ 6.2.1 ELECTION OF THE STEERING COMMITTEE

The Steering Committee is elected once a year in accordance with § 5.2.2. The election shall take place at the General Meeting. An adaptation of the "Majority Judgement"² is defined as the election system:

All MPG-affiliated individuals as defined in § 4 can run for election. Candidates for the Steering Committee shall opt for one of the three personnel categories at their own discretion before being elected:

- Scientific personnel
- Technical personnel
- Administrative personnel

To cover each of the three categories, at least one candidacy from each personnel category is desirable. Candidates can give reasons for their candidacy; academic titles and professional position within the MPG beyond these categories should not be mentioned. A gross violation may, at the discretion of the current Steering Committee, lead to exclusion from the election.

Afterwards all Local Chairs can express their opinion on each candidate by assigning them none (abstention) or one of the following mentions:

- Excellent
- Good
- Tolerable
- Insufficient
- Unacceptable (Rejection)

In order to ensure that all the categories of personnel are represented by at least one person, three candidates associated to the best median mention in each category as well as the two candidates with the best remaining medians across all categories are selected. These five elected members form the new Steering Committee. If two or more candidates have the same medians mention, median votes are progressively removed from candidates with the same median mentions until the median mentions become different and thus result in a decision.

The election will be conducted by the Working Group "Elections & Research" in close coordination with the current Steering Committee. Election results must be made publicly available. If the election is not held at the General Meeting, the current Steering Committee, in close coordination with the

² *PNAS* **2007**, 104 (21), 8720–8725. DOI: 10.1073/pnas.0702634104

“Elections & Research” Working Group, is obliged to present the exact procedure of the election at the General Meeting and to have it ratified by the General Meeting via an informal vote in accordance with § 6.3.1.

§ 6.2.2 ELECTION OF THE ADVISORY BOARD

The Advisory Board elections are held after the election of the new Steering Committee. There are three types of candidates who can be appointed to the Advisory Board for three years each:

1. Ordinary candidacy: Members of the outgoing Steering Committee who have not been re-elected may stand for election to the Advisory Board.
2. Extraordinary candidacy: As described in § 5.2.3, the current Steering Committee may propose (with scientific justification) individuals for extraordinary admission to the Advisory Board.
3. Re-election: After three years members of the Advisory Board can be re-elected. There are no restrictions on how often a person can be re-elected.

The Local Chairs can cast their votes to the candidates in the following categories:

- For
- Abstention
- Against

In order to be admitted to the Advisory Board, two conditions must be fulfilled for the candidate:

1. More than 25% vote for admission (the first quartile is "For")
2. Less than 25% vote against admission (the third quartile is not "Against")

If both conditions are met, the candidate is admitted to the Advisory Board for a period of three years. If one or more of the conditions are not met, the candidate is not admitted.

§ 6.2.3 RATIFICATION OF NEW STATUTES

The Steering Committee can create change proposals for these Statutes. The proposed changes must be communicated to the Local Chairs at least two weeks before the start of the General Meeting. The amendments must be discussed at the General Meeting. At the General Meeting, the proposals may be amended by informal voting in accordance with § 6.3.1 at the request of a person present at the General Meeting. In order to accept the amendments, a two-third majority of the Local Chairs entitled to vote is required.

§ 6.2.4 ELECTION REPRESENTATION OF THE CHAIR

If a Chair is unable to attend the General Meeting, the voting right can be transferred to a proxy by a written authorization. In addition to their own voting right, each Chair present at the General Meeting is entitled to vote with no more than one transferred voting right.

§ 6.3 INFORMAL VOTES AND ELECTIONS

The Informal Votes consist of the votes on motions proposed by the General Meeting and the election of the Working Group leaders. All members of the General Meeting are entitled to participate in the Informal Votes. Informal Votes can be conducted verbally or by show of hands.

§ 6.3.1 VOTES ON MOTIONS

At the discretion of the Steering Committee, an Informal Vote may be held immediately on a motion submitted by a member of the General Meeting. A successful proposal requires a simple majority of the votes of all members present at the General Meeting, in which case the proposal must be accepted. A motion may not be used to circumvent larger votes.

§ 6.3.2 ELECTION OF WORKING GROUP LEADERS

With the exception of the “Network & Report” Working Group, the members of each Working Group shall conduct an Informal Vote to elect the leader of that group. Each election requires a simple majority of the votes of the members of the group. The result is reported to the Steering Committee in order to be valid.

§ 7 ENTRY INTO FORCE

These Statutes will come into force the day after their publication through the communication channels of the Sustainability Network, after they have been discussed with the Sustainability Network and approved by the majority of the members of the Interim Steering Committee.

Negotiated by the Interim Steering Committee, December 17, 2019.

Changed by the 1st General Meeting, May 28, 2020.

APPENDIX 1 – ELECTION OF THE LOCAL CHAIRS – BEST PRACTICE RECOMMENDATION

The election as Chair of a local Sustainability Group should be open to all MPG-affiliated individuals as defined in § 4 - with the restriction of affiliation to the MPIs participating in the Sustainability Group. Accordingly, the call for candidates should be publicly accessible in writing to all members affiliated to the MPIs involved in the election at least two weeks before the election, with the announcement of the time and place of the election and a contact with the election management. This can be done by posting a notice at a central location or by e-mail. The candidacy should be possible for a period of at least three working days.

The election can be casted electronically or analogously. In any case, the election should be conducted anonymously. The legal and MPG-internal data protection regulations must be complied with. If necessary, the Steering Committee or the Working Group “Elections & Research” can be contacted for support.

MPG Members who are affiliated to several MPIs should decide at which MPI they wish to be eligible to vote before the election. The election of the Local Chairs of different MPIs can take place in the same ballot.

The election should be prepared and carried out by a committee consisting of at least two people which are not themselves eligible for election. The committee has the task of ensuring the legitimacy as well as the documentation of the election and forwarding the results to the Working Group “Elections & Research”. The results should include the following data:

- Names of the election committee

- Name(s) of the newly elected Local Chair(s)
- Assurance of the legitimacy of the election by the election committee
- Start of term of office for the Local Chairs (Term of office: 1 calendar year starting from acceptance of the election)
- Acceptance of the election by the newly elected Local Chair(s)

If a Local Chair leaves office prematurely, a new election shall be held. This is also the case if a Local Chair loses the status as MPG-affiliated individual as defined in § 4 or leaves the represented MPI for more than 4 months.

A2.8 An open letter to the Max Planck Society – appeal for nonbinary inclusive language. (English original + German translation incl. authors' comment)

9 April 2019

An open letter to the Max Planck Society

-Advance Copy-

The PhDnet Equal Opportunity Working Group is currently soliciting individual endorsements for this letter. It was provided to a group of central MPS administrators in mid-April, prior to a series of meetings in Munich about LGBTQ+ inclusion. After central administrators had an opportunity to read and endorse it, the letter and endorsement solicitation is now being broadly distributed to the MPS.

If you would like to add your name, email nonbinary@mpi-muelheim.mpg.de with your name/title, personal pronoun, position, and institute. You may also endorse anonymously or with any subset of this information.

Dear Max Planck Society,

We, the undersigned members of the Max Planck Society (MPS), are writing to politely but firmly request that the MPS recognize the existence, validity and right to an inclusive work environment of nonbinary people—those who do not self-identify as men or women. In this letter, we will offer a brief explanation of gender identity, demonstrate that inclusion of nonbinary identity is already well-underway within academia, and suggest the first steps to be taken by the MPS in achieving nonbinary inclusion.

Nonbinary Identity and Language

A nonbinary person can be defined quite simply: someone who is neither a man nor a woman. But to flesh out this definition, we must first establish concepts of gender and reproductive traits and the language of personal identity. (We write specifically about the English language; we do not take any position on the correspondence of these concepts to, for example, “Geschlecht.”)

Gender is a socio-psychological construction which may include traits of personality, psychology, and physical presentation such as clothing, as well as modes of interaction with society. A person’s gender is *how they feel and think about themselves*, and is completely *self-defined*. Reproductive traits are physical features of a body related to sexual reproduction, sometimes denoted collectively as a ‘biological sex.’ The words ‘man’ and ‘woman’, ‘he’ and ‘she,’ refer to gender, not reproductive traits. A person of any gender may have any combination of reproductive traits. For example, a transgender man is simply a man who was not assigned a male biological sex at birth. His self-identification as a man is precisely

what defines him as such and this identity does not require any external validation. The statement, “he identifies as a man,” is unnecessarily complicated (and to some, connotes an invalidating skepticism); one should simply write, “he is a man.”

A nonbinary person is neither a man nor a woman: they may have a gender that is a mixture of masculine and feminine or some third gender which is not describable in these terms, or they may be agender (not possessing any gender at all). As with men and women, nonbinary people may have any combination of reproductive traits. In the words of Robin Dembroff, “having an intersex condition is neither sufficient nor necessary for being nonbinary. The majority of nonbinary individuals do not have an intersex condition, nor do they take themselves to.” (The ‘d’ or ‘divers’ designation recently introduced in Germany is not an example of nonbinary acceptance, as it is defined by a medical evaluation of intersex reproductive traits, rather than anything related to gender.)

Nonbinary people often use pronouns which do not impose a binary gender. In English, we are fortunate to have a grammatically-established, non-gendered singular pronoun: the singular ‘they’ (see Appendix I).

I went to my doctor and they prescribed antibiotics.

Alex is a good cook; yesterday they made risotto.

“Everybody has their failing.” [Jane Austen]

“Now nobody does anything well that they cannot help doing.” [John Ruskin]

Despite this history and present usage, in certain contexts, some people find it difficult or awkward to use singular they. When one has previously known a particular person by a binary pronoun, it may take some time and effort to switch. This is okay, and the effort is worthwhile. Having coworkers and friends who use gender-appropriate language can be a powerfully affirming experience, while constant imposition of binary, misgendering language is emotionally taxing. Some of the undersigned, having come from more inclusive institutions, have felt isolation and invalidation in the MPS.

Nonbinary Identities Are Gaining Acceptance

Many institutions, organizations and governments have already taken significant steps towards accepting and including nonbinary people. See Appendix II for a partial list of supportive academic institutions.

The most prestigious universities in the United States, including Harvard, Yale, Stanford and the University of California, have adopted policies which allow self-identified community members to specify ‘nonbinary’ or ‘other’ as their gender

on internal documents, and are adopting cultures where singular ‘they’ pronouns are normalized. Ten states have adopted a nonbinary option for official identification (identification is issued by state governments in the US), available to anyone who self-identifies as nonbinary. This has compelled businesses which rely on government identification, such as airlines, to begin accommodating nonbinary gender as well.

In the UK, where formal titles are more widely used, the gender-neutral ‘Mx.’ is widely accepted in academic, governmental and financial institutions. For example, the University of Oxford “has amended its staff and student systems so that individuals can choose to be addressed by the title ‘Mx’.” As in the United States, many nonbinary people use the pronoun ‘they.’

Steps to Make the MPS a More Inclusive Institution

There are two categories of steps which would make the MPS a more inclusive place for nonbinary people: direct changes to administrative procedure and educational initiatives to improve workplace culture. We hope the following points will begin a practical dialog between central administration and the trans and nonbinary community of the MPS.

The first change to administration would be to include an option for ‘nonbinary’ or ‘other’ on any forms or databases which record gender. This must be self-identified, and not based on any government documents or medical diagnosis. In general, the term ‘gender’ must be used in a self-defined fashion, and not as a synonym for reproductive traits. If the ‘sex’ or ‘gender’ on someone’s official identification is required, this should be requested specifically, e.g. “sex or gender in the passport.” This will avoid confusion between governments with different levels of gender acceptance. (For example, US passports are only issuable with the sex assigned at birth and are not changed for state-recognized transgender people.) As the process of lying about one’s gender can be alienating, and as these forms and databases should be limited in number, we request this change be prioritized.

Other documents should be inclusive of all gender-binary and nonbinary people. While ‘he-or-she’ phrasing is some improvement over the old generic masculine, a contract that includes, “the researcher must keep his or her password secret,” does not include researchers who are neither ‘him’ nor ‘her.’ One should write, “the researcher must keep their password secret.” As this problem applies to many existing documents, we do not expect it to be solved quickly, but we request an official policy of using gender-neutral, nonbinary-inclusive language in all *new* documents.

While we believe uncompromisingly in the importance of nonbinary inclusion, we also recognize that these concepts are unfamiliar to some people and that significant effort will be required to establish the necessary conceptual and linguistic understanding. The MPS is a diverse institution including researchers from all over the world, and the translation of concepts such as ‘gender’ and ‘sex’ may be convoluted. But the project of meaningful inclusion is important: to feel one is part of a safe and inclusive community, one must be not merely tolerated, but understood by that community. We ask that the MPS work with nonbinary MPS members to develop educational materials, such as onboarding trainings and pamphlets, to be distributed to the institutes with the benefit of central administration approval. Such materials should establish the basic idea of self-defined gender and the imperative to respect the gender identities of all people.

In Conclusion

We, the undersigned, believe that, in order to foster a work environment that is inclusive to all, the Max Planck Society must recognize and accept nonbinary people, both formally and in workplace culture.

Sincerely,

Zachary S. Mathe, they | MSc student, MPI for Chemical Energy Conversion
Julian D. Rolfes, no pronoun preference | doctoral candidate, MPI for Coal Research
Erica McGale, they | doctoral candidate, MPI for Chemical Ecology

Endorsements:

Prof. Dr. Frank Neese, he | director, MPI for Coal Research
Prof. Dr. Serena DeBeer, she | director, MPI for Chemical Energy Conversion
Dr. Laure Decamps, she | group leader, MPI for Chemical Energy Conversion
Prof. Dr. Tobias Ritter | director, MPI for Coal Research
Dr. Aleksandra Wandzilak, she | postdoc, MPI for Chemical Energy Conversion
Dr. Bernadette Lessel | postdoc, MPI for the History of Science
Dr. Florian Kräutkli, he | research technology officer, MPI for the History of Science
Lindy Divarci | publication manager, MPI for the History of Science
Charlett Wenig | doctoral candidate, MPI of Colloids and Interfaces
Selina Carlhoff, she | doctoral candidate, MPI for the Science of Human History
Hannah Eßler, she | research assistant and student representative in questions of equality, MPI for the History of Science
Alina Topf | student assistant, MPI for the History of Science
Dr. Lisa Malich, she | junior professor and guest scientist, MPI for the History of

Science

Sean Wang, he | project manager, MPI for the History of Science; doctoral candidate, Syracuse University

Hannah Wiemer, she | guest postdoc, MPI for the History of Science; research fellow, Humboldt University

Dr. Ulla Weber, she | central gender equality officer, Human Resources Development & Opportunities, MPS Headquarters

Ms Frauke Logermann | senior consultant talent, gender & diversity, Human Resources Development & Opportunities, MPS Headquarters

Karen Giffin, she | doctoral candidate and local representative, MPI for the Science of Human History

Dr. Juliane Scholz, she | research associate, Research Project for the History of the MPS - GMPG, MPI for the History of Science

Dr. James A Daniel | project group leader, MPI of Experimental Medicine

Dr. Jacob Davidson | postdoc, MPI of Animal Behavior

Dr. Anneke M Batenburg, she | guest/former postdoc, MPI for Chemistry

Dr. Emiliano Zaccarella, he | group leader and postdoc representative, MPI for Human Cognitive and Brain Sciences

Dr. Erinn Gideons, she | postdoc, MPI for Experimental Medicine

Prof. Dr. Philipp Kanske | research associate, MPI for Human Cognitive and Brain Sciences

Dr. Sonja Schuh | IMPRS scientific coordinator, MPI for Solar System Research

Dr. Ursula Fünfschilling, she | gender equality officer, MPI for Coal Research

Simon M Hofmann | doctoral candidate and PhD representative, MPI for Human Cognitive and Brain Sciences

Gisela Govaart, she | doctoral candidate, MPI for Human Cognitive and Brain Sciences

Martin Grund, he | doctoral candidate, MPI for Human Cognitive and Brain Sciences

Maria Morozova | doctoral candidate and PhD representative, MPI for Human Cognitive and Brain Sciences

Katarzyna Gugnowska, she | doctoral candidate, MPI for Human Cognitive and Brain Sciences

Dr. Miriam Liedvogel, she | group leader, MPI for Evolutionary Biology

Dr. Martina Schlünder, she | research scholar, Research Project for the History of the MPS - GMPG, MPI for the History of Science

Dr. Michael Grange, he | postdoctoral fellow, MPI of Molecular Physiology

Prof. Dr. Paul B Rainey | director, MPI for Evolutionary Biology

Lic. Yennifer Hernandez, no pronoun preference | animal technician, MPI for Evolutionary Biology

Dr. Marianna Szczygielska, she | postdoctoral fellow, MPI for the History of Science

Dr. Liz Ing-Simmons, she | postdoc, MPI for Molecular Biomedicine

Dr. Amy Stetten, she | postdoc, MPI for Polymer Research

Dr. Rebecca McElroy, she | postdoc, MPI for Astronomy

Dr. Diane Feuillet, she | postdoc, MPI for Astronomy

Dr. Allison Merritt, she | postdoctoral fellow and postdoc representative, MPI for Astronomy

Dr. Elad Zinger, he | postdoc, MPI for Astronomy

Sarah Leslie, she | doctoral candidate, MPI for Astronomy

Dr. Néstor Espinoza, he | Bernoulli & IAU-Gruber Fellow, MPI for Astronomy

Melanie Kaasinen, she | doctoral candidate and gender equality officer, MPI for Astronomy

Vincent Carpenter, he | doctoral candidate, MPI for Astronomy

Dr. Saavidra Perera, she | postdoc, MPI for Astronomy

Stelios Lefkopoulos, he | doctoral candidate, MPI of Immunobiology & Epigenetics

Dr. David E. Sanin, he | postdoctoral research associate, MPI of Immunobiology & Epigenetics

Alexander Filippi, he | doctoral candidate and spokesperson of the Max Planck PhDnet, MPI for Chemistry

Johan Fridén, he | web designer, MPI of Immunobiology & Epigenetics

Dr. Michael Bartoschek, he | postdoc, MPI of Immunobiology & Epigenetics

David Marcolino Nielsen, he | doctoral candidate, IMPRS on Earth System Modelling, MPI for Meteorology

Louise Martens, she | doctoral candidate, MPI for Biological Cybernetics

Salvador Ramirez Acosta | doctoral candidate and member of LGBT+, MPI for the Structure and Dynamics of Matter

George Caputa, he/they | postdoc, MPI for Immunobiology & Epigenetics

Dr. Franco Bonafé, he | postdoc, MPI for the Structure and Dynamics of Matter

Dr. Silvia Caldararu, she | postdoc and gender equality officer, MPI for Biogeochemistry

Visnja Jevtic | technical assistant, MPI for Immunobiology & Epigenetics

Shane Stoner, he | doctoral candidate, MPI for Biogeochemistry

Martin Kunz, he | doctoral candidate, MPI for Biogeochemistry

Madeleine Bleasdale, she | doctoral candidate, MPI for the Science of Human History

Dr. Primrose Boynton, she | project leader, MPI for Evolutionary Biology

Dr. Ritwick Sawarkar, he | independent group leader, MPI for Immunobiology & Epigenetics

Mareike Neumann, she | doctoral candidate, MPI for Biogeochemistry

Marga Helene Pallandt, she | doctoral candidate and deputy gender equality officer, MPI for Biogeochemistry

Dr. Nikolay Kacharov, he | postdoc, MPI for Astronomy

David Martini, he | doctoral candidate, MPI for Biogeochemistry

Fabio Franzese, he | researcher, MPI for Social Law and Social Policy

Sanja Bökle | doctoral candidate, MPI for the Study of Religious and Ethnic Diversity

Dr. Jeremy F. Walton, he | research group leader, Empires of Memory: The Cultural

Politics of Historicity in Former Habsburg and Ottoman Cities, MPI for the Study of Religious and Ethnic Diversity

Dr. Kristin Futterlieb, she | head librarian, MPI for the Study of Religious and Ethnic Diversity

Evelyn Medawar, she | doctoral candidate, MPI for Human Cognitive and Brain Sciences

Geet George, they | doctoral candidate, MPI for Meteorology

Amy Foster, she | MSc student, MPI of Molecular Plant Physiology

Dr. Valérie Hilgers, she | research group leader and deputy gender equality officer, MPI of Immunobiology & Epigenetics

Laura Lambert, she | doctoral candidate, MPI for Social Anthropology

S. Martin, she | doctoral candidate, MPI for Human Cognitive and Brain Sciences

Jan Brüwer, he | doctoral candidate, MPI for Marine Microbiology

Lydi(a) Keppler, she | doctoral candidate, MPI for Meteorology

Çağlar Küçük, they | doctoral candidate, MPI for Biogeochemistry

Grace Ho, she | MSc student, MPI for Marine Microbiology

Patrick Barth, he | MSc student, MPI for Astronomy

Davide Silvagni, he | doctoral candidate, MPI for Plasma Physics

Robert Stendel, he | research fellow and doctoral candidate, MPI for Comparative Public Law and International Law

Karl Stimmel | doctoral candidate, MPI for Plasma Physics

Jan Gerken, he | doctoral candidate, MPI for Gravitational Physics (AEI)

Johanna Gebhard, she | doctoral candidate, MPI for Marine Microbiology

Anonymous, they | doctoral candidate, MPI for Marine Microbiology

Henrique Valim, he | doctoral candidate, MPI for Chemical Ecology

Frederik Busse, he | doctoral candidate, MPI for the Structure and Dynamics of Matter

Julia Misersky, she | doctoral candidate and PhD representative, MPI for Psycholinguistics Nijmegen (NL)

Dr. Megha Amrith, she | group leader, MPI for the Study of Religious and Ethnic Diversity

Dr. Kok Leng Yeo, she | postdoc, MPI for Solar System Research

Dr. Ana Vila Verde, she | group leader and gender equality officer, MPI of Colloids and Interfaces

Lucas Kuhrts | doctoral candidate, MPI of Colloids and Interfaces

Ricardo Ziege | doctoral candidate, MPI of Colloids and Interfaces

Prof. Dr. Caroline Rowland, she | director, MPI for Psycholinguistics

Dr. Cécile Bidan, she | group leader, MPI of Colloids and Interfaces

Dr. Frank Ohme, he | group leader, MPI for Gravitational Physics (AEI)

Dr. Ro Jefferson, they | postdoc, MPI for Gravitational Physics (AEI)

Dr. Tom Robinson | group leader, MPI of Colloids and Interfaces

Dr. Stephan Eickelmann, he | postdoc, MPI of Colloids and Interfaces

Corentin Gut | guest doctoral candidate, MPI for Gravitational Physics (AEI) and
Leibniz University Hannover Institute of Theoretical Physics

Dr. Laurel Brehm, she | postdoc, MPI for Psycholinguistics

Dr. Evan Kidd, no preference | group leader, MPI for Psycholinguistics

Dr. Andrea E. Martin, she | group leader, MPI for Psycholinguistics; principal
investigator, Donders Centre for Cognitive Neuroimaging, Radboud
University

Dr. Andrew Matas, he | postdoc, MPI for Gravitational Physics (AEI)

Dr. M. Alessandra Papa, she | independent research group leader, MPI for
Gravitational Physics (AEI)

Frederic Nowak | doctoral candidate, MPI of Animal Behavior

Christina Bergmann, she | research staff, MPI for Psycholinguistics

Limor Raviv, she | doctoral candidate, MPI for Psycholinguistics

Alessio Quaresima, he | doctoral candidate, MPI for Psycholinguistics Nijmegen

Katja Stärk, she | doctoral candidate, MPI for Psycholinguistics

Dr. Reinhard Prix, he | staff scientist, MPI for Gravitational Physics (AEI)

Eirini Zormpa, she | doctoral researcher, MPI for Psycholinguistics Nijmegen

Jeroen van Paridon, he | doctoral candidate, MPI for Psycholinguistics

Aroma Dabas, she | doctoral researcher, MPI for Cognitive and Brain Sciences

Dr. Lukas Maes, he | postdoc, MPI for Solar System Research

Dr. Christine Gieraths, she | senior officer, Department of Research Policy and
External Relations, MPS Headquarters

Dr. Jan Steinhoff, he | group leader, MPI for Gravitational Physics (AEI)

*If you would like to add your name, email nonbinary@mpi-muelheim.mpg.de with
your name/title, personal pronoun, position, and institute. You may also endorse
anonymously or with any subset of this information.*

Appendix I: Further Reading

Understanding Non-Binary People: How to Be Respectful and Supportive | NCTE

An overview of nonbinary identity from the National Center for Transgender Equality in the United States

www.transequality.org/issues/resources/understanding-non-binary-people-how-to-be-respectful-and-supportive

Resources | Gender Identity Research & Education Society

A collection of educational and practical resources for gender-nonconforming people in the UK

www.gires.org.uk/resources/

Trans Awareness | Equality, diversity and inclusion, Imperial College London

A set of administrative guidelines for trans and nonbinary inclusion; Section 8 of the Trans Staff Policy provides exemplary pronoun guidelines.

www.imperial.ac.uk/equality/support-for-staff/resources/trans-awareness/

Gender-neutral titles | The Equality & Diversity Unit, University of Oxford

A brief explanation of gender-neutral titles in the UK and at the University of Oxford

www.admin.ox.ac.uk/eop/transgender/gender-neutraltitles

Singular ‘They’ | Editors, Merriam-Webster English Dictionary

Editors of the oldest American English dictionary describe the use of singular ‘they,’ both for persons of contextually-undefined gender and nonbinary people.

www.merriam-webster.com/words-at-play/singular-nonbinary-they

A brief history of singular ‘they’ | Denis Baron, Oxford English Dictionary

Baron, professor of English and linguistics at the University of Illinois, lays out the history of ‘they’ as a pronoun referring to a single person.

public.oed.com/blog/a-brief-history-of-singular-they

Why be Nonbinary? | Robin Dembroff, Aeon

Dembroff, assistant professor of philosophy at Yale, deconstructs gender and describes the liberatory potential of “[embracing] an ontological space outside the gender binary.”

aeon.co/essays/nonbinary-identity-is-a-radical-stance-against-gender-segregation

Appendix II: Partial List of Academic Institutions with Nonbinary-Inclusive Policies

Harvard University
Yale University
University of California
Stanford University
California Institute of Technology
University of Chicago
Reed College
Cornell University
Princeton University
University of Michigan
Carleton College
University of Wisconsin
Amherst College
University of Vermont

University of Oxford
Imperial College London
London School of Economics
University of Exeter
University College London
Edinburgh University
Durham University
University of Warwick

9. April 2019

Offener Brief an die Max-Planck-Gesellschaft (Ins Deutsche übersetzt durch Jessica Sutter, Julian D. Rolfes, Ruth Ley & Birgit Moldovan)

-Vorabexemplar-

Die Phdnet-Arbeitsgruppe für Chancengleichheit bemüht sich zurzeit um persönliche Unterstützung für dieses Schreiben. Es wurde Mitte April im Vorfeld einer Reihe von Besprechungen zum Thema LGBTQ+-Inklusion einem Teil der Generalverwaltung der MPG vorgelegt. Nachdem die Mitglieder der Generalverwaltung die Gelegenheit hatten, es zu lesen und zu befürworten, wird das Schreiben und das Ersuchen um Unterstützung jetzt flächendeckend an die MPG verteilt.

Wenn Sie das Schreiben unterzeichnen möchten, senden Sie bitte eine E-Mail mit Ihrem Namen/Titel, dem Personalpronomen, der Position und dem Institut an nonbinary@mpi-muelheim.mpg.de. Sie können das Anliegen auch anonym oder mit einem Teil dieser Angaben befürworten.

Sehr geehrte Max-Planck-Gesellschaft,

wir, die unterzeichneten Mitglieder der Max-Planck-Gesellschaft, möchten Sie mit diesem Schreiben höflich, aber mit Nachdruck, ersuchen, dass die MPG die Existenz, die Berechtigung und das Recht auf eine inklusive Arbeitsumgebung für nichtbinäre Menschen – die sich weder als männlich noch als weiblich identifizieren – anerkennt. In diesem Schreiben werden wir die Genderidentität kurz erläutern, aufzeigen, dass die Inklusion der nichtbinären Identität in der akademischen Welt bereits in vollem Gange ist sowie erste Schritte empfehlen, die von der MPG zur Umsetzung einer Nichtbinär-Inklusion zu ergreifen sind.

Nichtbinäre Identität und Sprache

Eine nichtbinäre Person kann einfach als eine Person definiert werden, die weder Mann noch Frau ist. Um diese Definition zu konkretisieren, müssen wir jedoch zunächst Konzepte von Gender und Fortpflanzungsmerkmalen und die Sprache der persönlichen Identität beleuchten. (Wir äußern uns speziell zur englischen Sprache. Für weitere Erläuterungen zum Lösungsansatz für die deutsche Sprache beachten Sie bitte die Kommentare der Autor*innen am Ende dieses Dokuments.)

Gender ist ein soziopsychologisches Konstrukt, das Merkmale der Persönlichkeit, Psychologie und physischen Präsentation, wie beispielsweise Kleidung, sowie Arten der Interaktion mit der Gesellschaft beinhalten kann. Das Gender einer Person besagt, *wie sie sich fühlt und über sich denkt*, und ist vollkommen *selbstdefiniert*. Fortpflanzungsmerkmale sind physische Merkmale eines Körpers, die mit der sexuellen Fortpflanzung zusammenhängen und bisweilen kollektiv als „biologisches Geschlecht“ bezeichnet werden. Die Wörter „Mann“ und „Frau“, „er“ und „sie“

beziehen sich auf Gender, nicht auf Fortpflanzungsmerkmale. Eine Person eines bestimmten Genders kann eine beliebige Kombination von Fortpflanzungsmerkmalen aufweisen. Beispielsweise ist ein Transgender-Mann ein Mann, dem bei seiner Geburt kein männliches biologisches Geschlecht zugewiesen wurde. Seine Selbstidentifikation als Mann ist das, was ihn als solchen definiert, und diese Identität erfordert keine externe Validierung. Die Aussage „Er identifiziert sich als Mann“ ist unnötig kompliziert (und impliziert für manchen eine disqualifizierende Skepsis). Stattdessen sollte man schreiben: „Er ist ein Mann.“

Eine nichtbinäre Person ist weder ein Mann noch eine Frau. Sie kann ein Gender aufweisen, das eine Mischung aus maskulin und feminin oder ein bestimmtes drittes Geschlecht darstellt, das sich in diesen Begriffen nicht beschreiben lässt, oder sie besitzt überhaupt kein Gender (ein Agender). Wie Männer und Frauen können auch nichtbinäre Menschen eine Kombination aus Fortpflanzungsmerkmalen aufweisen. Um mit Robin Dembroff zu sprechen, „ein intersexueller Zustand ist weder ausreichend noch notwendig, um nichtbinär zu sein. Die Mehrzahl der nichtbinären Personen weist keinen intersexuellen Zustand auf und nimmt diesen nicht für sich in Anspruch.“ (Die Bezeichnung „d“ oder „divers“, die kürzlich in Deutschland eingeführt wurde, ist kein Beispiel für nichtbinäre Akzeptanz, da sie durch eine medizinische Beurteilung intersexueller Fortpflanzungsmerkmale definiert wird und nicht durch einen Aspekt in Verbindung mit Gender.)

Nichtbinäre Menschen verwenden häufig Pronomen, die kein binäres Gender beschreiben. Im Englischen haben wir glücklicherweise ein grammatikalisch etabliertes, nicht genderspezifisches Singularpronomen: die Singularform „they“ (siehe Anhang I).

*I went to my doctor and “they” prescribed antibiotics.
(Ich ging zum Arzt und „they“ verschrieb Antibiotika.)
Alex is a good cook; yesterday “they” made risotto.
(Alex ist ein guter Koch. Gestern machte “they” Risotto.)*

Trotz der historischen und gegenwärtigen Verwendung in bestimmten Kontexten empfinden es manche Menschen als schwierig oder umständlich, „they“ als Singular zu verwenden. Wenn jemand eine bestimmte Person bislang durch ein binäres Pronomen bezeichnet hat, kann es etwas Zeit und Mühe kosten umzuschalten. Das ist in Ordnung, und es ist die Mühe wert. Wenn man Kolleg*innen und Freunde hat, die eine gender-adäquate Sprache verwenden, kann dies als starke Bestätigung erlebt werden. Eine konstant aufgezwungene binäre, das falsche Gender zuweisende Sprache ist hingegen emotional belastend. Einige der Unterzeichneten, die aus inklusiveren Institutionen kommen, haben in der MPG Isolation und Disqualifizierung verspürt.

Nichtbinäre Identitäten gewinnen an Akzeptanz

Viele Institutionen, Organisationen und Regierungen haben bereits signifikante Schritte auf dem Weg zu Akzeptanz und Einbeziehung nichtbinärer Menschen unternommen. In Anhang II der englischen Version findet sich eine Liste wissenschaftlicher Institutionen, die diese Grundsätze bereits unterstützen.

Die angesehensten Universitäten in den Vereinigten Staaten, einschließlich Harvard, Yale, Stanford und der University of California, haben Richtlinien eingeführt, die es den selbstidentifizierten Community-Mitgliedern ermöglichen, in internen Dokumenten „nichtbinär“ oder „sonstiges“ als ihr Gender anzugeben, und etablieren eine Kultur, in der das Singularpronomen „they“ zur Norm wird. Zehn Staaten haben eine nichtbinäre Option für offizielle Ausweisdokumente eingeführt (Ausweise werden in den USA durch die Regierungen der Einzelstaaten ausgegeben), die jedem zur Verfügung steht, der sich selbst als nichtbinär identifiziert. Dies hat Unternehmen, die auf staatliche Ausweisdokumente zurückgreifen, wie beispielsweise Fluglinien, gezwungen, das nichtbinäre Gender ebenfalls zu übernehmen.

Im Vereinigten Königreich, wo die formale Anrede stärker verbreitet ist, wird das genderneutrale „Mx“ in wissenschaftlichen und staatlichen Institutionen und Finanzinstituten weitreichend akzeptiert. Die University of Oxford hat beispielsweise „ihre Personal- und Studierendensysteme so geändert, dass Einzelpersonen sich entscheiden können, mit der Anrede „Mx“ angesprochen zu werden“. Wie in den Vereinigten Staaten verwenden auch dort viele Menschen das Pronomen „they“.

Maßnahmen, um die MPG zu einer inklusiveren Institution zu machen

Es gibt zwei Kategorien von Maßnahmen, um die MPG zu einem inklusiveren Ort für nichtbinäre Menschen zu machen: direkte Änderungen bezüglich Verwaltungsverfahren sowie Schulungsinitiativen, um die Kultur am Arbeitsplatz zu verbessern. Wir hoffen, mit den folgenden Punkten einen pragmatischen Dialog zwischen der zentralen Verwaltung und der Trans- und Nichtbinär-Community der MPG anzustoßen.

Die erste Änderung in der Verwaltung wäre die Einbeziehung einer Option für „nichtbinär“ oder „sonstiges“ in alle Formulare oder Datenbanken, in denen das Gender erfasst wird. Das Gender muss selbstidentifiziert sein und nicht auf staatlichen Dokumenten oder medizinischen Diagnosen basieren. Im Allgemeinen muss der Begriff „Gender“ gemäß Selbstdefinition verwendet werden und nicht als Synonym für Fortpflanzungsmerkmale. Wenn das „Geschlecht“ oder „Gender“ aus offiziellen Ausweisdokumenten einer Person erforderlich ist, sollte dies speziell angegeben werden, z. B. „Geschlecht oder Gender im Reisepass“. Dadurch werden Missverständnisse zwischen Staaten mit verschiedenen Ebenen der Gender-akzeptanz vermieden. (US-Pässe werden beispielsweise nur mit dem bei Geburt zugewiesenen

Geschlecht ausgegeben und für staatlich anerkannte Transgender-Menschen nicht geändert.) Da das Verschweigen des eigenen Genders zu Entfremdung führen kann, und da diese Formulare und Datenbanken zahlenmäßig begrenzt sein dürften, beantragen wir eine Priorisierung dieser Änderung.

Andere Dokumente sollten alle Gender einbeziehen - binäre und nichtbinäre Personen. Wenngleich die Formulierung „er oder sie“ eine gewisse Verbesserung gegenüber dem alten generischen Maskulin darstellt, bezieht ein Vertrag, der besagt, dass „der Forscher oder die Forscherin sein oder ihr Passwort geheim halten muss“, keine Forscher*innen ein, die weder „er“ noch „sie“ sind. Man sollte dies eher so formulieren: „Forscher*innen müssen ihr Passwort geheim halten“. Da dieses Problem für viele bestehende Dokumente gilt, gehen wir nicht davon aus, dass es schnell gelöst wird. Wir erbitten jedoch eine offizielle Richtlinie zur Verwendung einer genderneutralen, nichtbinär-inklusiven Sprache in allen *neuen* Dokumenten.

Wenngleich wir von der Bedeutung der Nichtbinär-Inklusion absolut überzeugt sind, können wir nachvollziehen, dass diese Konzepte für manche Menschen ungewohnt sind, und dass ein signifikanter Einsatz erforderlich sein wird, um das notwendige konzeptionelle und sprachliche Verständnis zu etablieren.

Die MPG ist eine facettenreiche Institution, die Forscher*innen aus aller Welt umfasst, und die Umsetzung von Konzepten wie „Gender“ und „Geschlecht“ kann kompliziert sein. Aber das Projekt einer sinnvollen Inklusion ist wichtig: Um das Gefühl zu haben, dass man einer sicheren und inklusiven Gemeinschaft angehört, muss man von dieser Gemeinschaft nicht nur toleriert, sondern auch verstanden werden. Wir ersuchen die MPG, mit nichtbinären MPG-Mitgliedern zusammenzuarbeiten, um Schulungsmaterialien zu entwickeln, beispielsweise Onboarding-Trainings und Broschüren, die mit Genehmigung der Generalverwaltung an die Institute verteilt werden; diese sollen dazu dienen, das Grundkonzept des selbstidentifizierten Genders zu etablieren, um somit zu gewährleisten, dass den Genderidentitäten aller Menschen mit unabdingbarem Respekt begegnet wird.

Schlussfolgerung

Wir, die Unterzeichneten, sind überzeugt, dass die Max-Planck-Gesellschaft eine Arbeitsumgebung fördern sollte, die für alle inklusiv ist, und daher nichtbinäre Menschen anerkennen und akzeptieren muss – formal und in der Kultur am Arbeitsplatz.

Mit freundlichen Grüßen,

Zachary S. Mathe, they | MSc Student, MPI for Chemical Energy Conversion
Julian D. Rolfes, no pronoun preference | doctoral candidate, MPI for Coal Research
Erica McGale, they | doctoral candidate, MPI für Chemical Ecology

Wenn Sie Ihren Namen hinzufügen möchten, senden Sie bitte eine E-Mail mit Ihrem Namen/Titel, dem Personalpronomen, der Position und dem Institut an nonbinary@mpi-muelheim.mpg.de. Sie können das Anliegen auch anonym oder mit einem Teil dieser Angaben befürworten. Die Liste der Unterstützenden ist der englischen Originalversion angehängt.

Anhang I: Literaturhinweise

Understanding Non-Binary People: How to Be Respectful and Supportive | NCTE

Eine Übersicht zur nichtbinären Identität vom National Center for Transgender Equality in den Vereinigten Staaten

www.transequality.org/issues/resources/understanding-non-binary-people-how-to-be-respectful-and-supportive

Resources | Gender Identity Research & Education Society

Eine Zusammenstellung schulungsrelevanter und praktischer Ressourcen für gender-nichtkonforme Menschen im Vereinigten Königreich

www.gires.org.uk/resources/

Trans Awareness | Equality, diversity and inclusion, Imperial College London

Eine Reihe administrativer Leitlinien für Trans- und Nichtbinär-Inklusion, Kapitel 8 der Trans-Personal-Richtlinie liefert Beispiele für die Pronomenverwendung.

www.imperial.ac.uk/equality/support-for-staff/resources/trans-awareness/

Gender-neutral titles | The Equality & Diversity Unit, University of Oxford

Eine kurze Erklärung genderneutraler Anreden im Vereinigten Königreich und an der University of Oxford

www.admin.ox.ac.uk/eop/transgender/gender-neutraltitles

Singular 'They' | Editors, Merriam-Webster English Dictionary

Die Herausgeber des ältesten Wörterbuchs für amerikanisches Englisch beschreiben die Verwendung der Singularform „they“ für Personen mit kontextuell undefiniertem Gender und nichtbinäre Personen.

www.merriam-webster.com/words-at-play/singular-nonbinary-they

A brief history of singular 'they' | Denis Baron, Oxford English Dictionary

Baron, Professor für Englisch und Linguistik an der University of Illinois, beleuchtet die Geschichte von „they“ als Pronomen, das sich auf eine einzige Person bezieht.

public.oed.com/blog/a-brief-history-of-singular-they

Why be Nonbinary? | Robin Dembroff, Aeon

Dembroff, Hochschuldozent für Philosophie in Yale, dekonstruiert Gender und beschreibt das befreiende Potenzial der „[Akzeptanz] eines ontologischen Raums außerhalb der Genderbinarität“.

aeon.co/essays/nonbinary-identity-is-a-radical-stance-against-gender-segregation

Anhang II: Unvollständige Liste der wissenschaftlichen Institutionen mit nichtbinär-inklusiven Richtlinien

Harvard University
Yale University
University of California
Stanford University
California Institute of Technology
University of Chicago
Reed College
Cornell University
Princeton University
University of Michigan
Carleton College
University of Wisconsin
Amherst College
University of Vermont

University of Oxford
Imperial College London
London School of Economics
University of Exeter
University College London
Edinburgh University
Durham University
University of Warwick

Zusätzlicher Kommentar der Autor*innen zum Brief:

Dass sich der vorliegende Brief trotz des zweisprachigen Ansatzes der Max-Planck-Gesellschaft lediglich auf die englische Sprache bezieht, liegt vor allem begründet in dem klaren Lösungsansatz, den die englische Sprache bietet (das ‚singular they‘). In der deutschen Sprache besteht jedoch eine andere Ausgangslage; die deutsche Sprache ist hochgradig segregiert in männliche und weibliche Formen der berufsbezeichnenden und beschreibenden Substantive, die sich auf Personen beziehen (Lehrer/Lehrerin, Student/Studentin, Mitarbeiter/Mitarbeiterinnen, Direktoren/Direktorinnen, ...). Aufgrund dessen besteht eine Vielzahl von mehr oder weniger inklusiven Ansätzen der geschlechtergerechten Sprache. Die am wenigsten inklusive ist dabei vermutlich das generische Maskulinum, welches nahezu ausschließlich im Verlauf der vergangenen Jahrhunderte Verwendung fand.

Wir bedauern, dass es zum jetzigen Zeitpunkt keine offizielle Form der geschlechtergerechten deutschen Sprache gibt. Dies liegt unserer Ansicht nach unter anderem darin begründet, dass bisher noch keine optimale Lösung vorliegt. Es existiert auch eine Reihe geschlechter-neutraler Pronomen¹, davon hat sich zum jetzigen Zeitpunkt aber noch kein Vorschlag durchgesetzt. Dennoch möchten wir gerne aus dem Pool der bestehenden Formen der geschlechtergerechten Sprache eine Version herausstellen, die unserer Ansicht nach² den derzeit besten Kompromiss aus Praktikabilität und Inklusion bildet:

Sofern möglich, ist ein substantiviertes Partizip (z.B. ‚Studierende‘, ‚Mitarbeitende‘) eine elegante Lösung.³ In manchen Fällen kann für Personengruppen auf ein neutrales Substantiv zurückgegriffen werden (z.B. ‚Direktorium‘, ‚Kollegium‘, ‚Lehrkörper‘, ‚technisches/administratives/wissenschaftliches Personal‘). In den Fällen, in denen ein substantiviertes Partizip zu sperrig oder unpraktikabel ist (z.B. ‚Zurschulegehende‘) und kein neutrales Substantiv zur Verfügung steht, sprechen wir uns für die Benutzung des **generischen Femininums in Zusammenhang mit dem Genderstern** aus: „Wir sind auf der Suche nach einer engagierten Student*in.“ Wir erkennen die Kritik an der Disruption der Substantive an, halten es jedoch – z.B. im Vergleich zum weniger disruptiven Binnen-I (‚StudentIn‘, ‚DirektorInnen‘) – für den inklusiveren Lösungsansatz, da auch nichtbinäre Mitglieder der Gesellschaft sprachlich integriert werden. Die Wahl des generischen Femininums erleichtert dabei die Form der vorangestellten Artikel und Pronomen sowie den Lesefluss maßgeblich.

Mit Blick auf die Entwicklung der geschlechtergerechten Sprache schließen wir uns dem Vorschlag der feministischen Linguistin Luise F. Pusch an,⁴ einen weiteren Buchstaben auf der deutschen Tastatur (analog zu @ und €) einzuführen; das ‚Gender-i‘. Dieses würde den Genderstern anstelle des i-Punktes in den Buchstaben integrieren und somit die Disruption des Wortes vermeiden.

¹ <https://nibi.space/pronomen>

² Dies entspricht lediglich der Ansicht der Autor*innen, nicht notwendigerweise der Unterstützenden.

³ Der Kritik, dass Studierende streng genommen nur studierend sind in den Momenten, in denen sie studieren, (schlafende Studierende also streng genommen Schlafende sind,) sei die Wortherkunft ‚studens‘ – ‚studierend‘ (also ein lateinisches Partizip) des Wortes ‚Studentin‘ gegenübergestellt.

⁴ <https://www.jetzt.de/hauptsache-gendern/gendern-linguistin-luise-f-pusch-ueber-das-gendersternchen-und-geschlechtergerechte-sprache>

**A2.9 “Aufruf zur Selbstverpflichtung der Mitarbeitenden der
Max-Planck-Gesellschaft: Klimafreundliche Dienstreisen / Call for
Voluntary Commitment by the Coworkers of the Max Planck
Society: Climate-Friendly Business Trips”**

Aufruf zur Selbstverpflichtung der Mitarbeitenden der Max-Planck-Gesellschaft: Klimafreundliche Dienstreisen

Der Besuch von Konferenzen sowie die Durchführung von Projekten mit bundesweiten und internationalen Partner*innen ist einerseits bereichernd und trägt zur wissenschaftlichen Verständigung und Problemlösung bei, andererseits gehen die damit verbundenen Reisen aber mit erheblichen CO₂-Belastungen einher.

Bei der Wahl des Verkehrsmittels sollten neben Aspekten wie Entfernung, Zeit, Machbarkeit und Kosten auch die CO₂-Emissionen eine wichtige Rolle spielen. Bahn und andere öffentliche Verkehrsmittel weisen eine deutlich bessere CO₂-Bilanz auf als PKW oder Flugzeug.

Flüge sind durch den Höheneffekt besonders klimaschädlich und in Deutschland für fast 10% des Effekts von Emissionen von Treibhausgasen verantwortlich [1]. Die ETH Zürich hat festgestellt, dass die Hälfte ihrer Treibhausgas-Emissionen von Flugdienstreisen verursacht ist [2]. Kurzstreckenflüge sind besonders leicht durch Bahnreisen zu ersetzen, je nach Strecke verursacht eine Standard-Bahnreise um die 10% der Emissionen eines entsprechenden Flugs [3]. Das bahn.business-Programm der Deutschen Bahn, an dem auch die MPG teilnimmt, verspricht durch 100% Ökostrom und Kompensation der indirekten Emissionen durch atmosfair sogar Klimaneutralität [4].

Ein notwendiger Schritt, um deutlich zum Klimaschutz beizutragen, ist die Vermeidung von Kurzstreckenflügen. Zu den Kurzstrecken rechnen wir Reisen unter 1000 km Entfernung, sofern diese mit der Bahn in weniger als 12 Stunden abgeschlossen werden können. **Wir verpflichten uns, auf vermeidbare Kurzstreckenflüge zu verzichten** und rufen die Generalverwaltung der Max-Planck-Gesellschaft sowie die Direktorien der Max-Planck-Institute dazu auf, mögliche Mehrkosten durch die Vermeidung von Kurzstreckenflügen zu übernehmen.

Ein weiterer wichtiger Schritt ist die Kompensation von unvermeidbaren Flugreisen durch die Finanzierung von ausgleichenden Klimaschutzmaßnahmen. Wir erkennen die aktuellen Bemühungen der Generalverwaltung an, die Legitimierung der Kompensation zu erwirken und freuen uns über die federführende Rolle der Max-Planck-Gesellschaft.

Call for Voluntary Commitment by the Coworkers of the Max Planck Society: Climate-Friendly Business Trips

Attending conferences as well as conducting projects with national and international partners is on the one hand enriching and contributes to scientific understanding and problem solving, but on the other hand the associated trips are associated with considerable CO₂ emissions.

When choosing a means of transport, CO₂ emissions should play an important role in addition to aspects such as distance, time, feasibility and costs. The CO₂ balance of rail and other public transport is significantly better than that of cars or planes.

Due to the effect of altitude, flights are particularly harmful to the climate and account for almost 10% of the greenhouse gas emissions effect in Germany [1]. ETH Zurich has determined that half of their greenhouse gas emissions are caused by flight duty travel [2]. Short-haul flights are particularly easy to replace by train travel, depending on the route causes a train journey to the 10% emissions of a corresponding flight [3]. Deutsche Bahn's bahn.business programme, in which the MPG also participates, even promises climate neutrality through 100% green electricity and compensation for indirect emissions through atmosfair [4].

A necessary step to make a significant contribution to climate protection is to avoid short-haul flights. We include journeys of less than 1000 km in the short-haul category if they can be completed by train in less than 12 hours. **We commit to refrain from avoidable short-haul flights** and call on the General Administration of the Max Planck Society as well as the Directorates of the Max Planck Institutes to cover possible additional costs by avoiding short-haul flights.

Another important step is to compensate for unavoidable air travel by financing compensatory climate protection measures. We recognize the current efforts of the General Administration to legitimize the compensation and are pleased about the leading role of the Max Planck Society.

Auszug aus dem Bundesreisekostengesetz (BRKG) / Excerpt from the Bundesreisekostengesetz (BRKG):

Deutsche Originalversion [5]:

§ 4 Fahrt- und Flugkostenerstattung

(1) Entstandene Kosten für Fahrten auf dem Land- oder Wasserweg mit regelmäßig verkehrenden Beförderungsmitteln werden bis zur Höhe der niedrigsten Beförderungsklasse erstattet. Für Bahnfahrten von mindestens zwei Stunden können die entstandenen Fahrtkosten der nächsthöheren Klasse erstattet werden. Wurde aus dienstlichen oder wirtschaftlichen Gründen ein Flugzeug benutzt, werden die Kosten der niedrigsten Flugklasse erstattet. Kosten einer höheren Klasse regelmäßig verkehrender Beförderungsmittel können erstattet werden, wenn dienstliche Gründe dies im Einzelfall oder allgemein erfordern.

English Translation:

§ 4 Reimbursement of travel and flight expenses

(1) Costs incurred for journeys by land or water with regularly operating means of transport shall be reimbursed up to the amount of the lowest transport class. For rail journeys of at least two hours, the travel costs incurred for the next higher class may be reimbursed. If an aircraft has been used for business or economic reasons, the costs of the lowest flight class will be reimbursed. Costs of a higher class of regular means of transport may be reimbursed if this is required for business reasons in individual cases or in general.

Auszug aus der Stellungnahme der Generalverwaltung der MPG / Excerpt from the Statement of the General Administration of the MPS:

Deutsche Originalversion:

Mit Datum vom 21. Januar 2020 hat die Dienstrechtsabteilung D 6 des Bundesministeriums des Innern, für Bau und Heimat im Rahmen einer Vorgriffsregelung mitgeteilt, dass **mit sofortiger Wirkung Dienstreisenden die Kosten einer Bahnfahrt auf freiwilliger Basis auch dann erstattet werden, wenn die Dienstreise dadurch teurer wird und länger dauert, als bei Nutzung eines Fluges**. Dies beinhaltet auch zusätzlich anfallende Übernachtungs- und Tagesgelder.

Damit wird ein erster Schritt zur Umsetzung des im Klimaschutzprogramm 2030 der Bundesregierung enthaltenen Punktes 3.5.1.3 „Minderung von Emissionen aus Dienstreisen“ getan. [...]

Für neu zu beantragende Dienstreisen wird die Reisestelle, soweit die Nutzung der Bahn vom Dienstreisenden gewünscht ist, nicht auf ein wirtschaftlicheres Angebot von Fluggesellschaften verweisen.

Vor der Beantragung von Bahnreisen als Alternative zum Flug ist der Reiseablauf am Institut mit dem jeweiligen Vorgesetzten abzustimmen. Dies insbesondere dann, wenn eine deutliche Verlängerung von ein bis maximal zwei Tagen der Reisezeit durch die Bahnnutzung entsteht. So lassen sich spätere Stornokosten vermeiden. Eine darüber hinaus gehende Verlängerung der Dienstreise ist nicht mehr vertretbar.

Alle Bahntickets, die über ORBS gebucht werden, sind „Grüne Tickets“ und bedürfen daher keiner weiteren Kompensation. Freiwillige Zahlungen für Flugkompensationen sind derzeit keine notwendigen Reisekosten und werden daher nicht erstattet.

Für Reisen mit dem privaten KFZ nach § 5 BRKG können freiwillig geleistete CO₂-Kompensationszahlungen auf der Basis einer Regelkompensation ab sofort im Rahmen der Reisekostenabrechnung als Nebenkosten nach § 10 BRKG erstattet werden. Die Erstattung von Kompensationszahlungen für Reisen mit dem Dienst-KFZ ist ausgeschlossen. Zusatzspenden über die Regelberechnung hinaus werden nicht erstattet.

Das Rundschreiben des BMI ist so auszulegen, dass in jedem Fall der Beschäftigte selbst die CO2-Kompensation veranlassen muss, nicht die Reisestelle. Das dann erhaltene Zertifikat ist zusammen mit der Reisekostenabrechnung einzureichen. Dieses Verfahren ist für jede einzelne Dienstreise anzuwenden und schließt damit eine gesammelte Kompensationszahlung (z. B. am Jahresende) aus.

Da noch keine geeignete behördenseitige Plattform für die Berechnung der notwendigen Regelkompensation existiert, kann der Dienstreisende frei wählen, bei welcher Institution er seine Kompensationszahlung leistet, hier bietet sich beispielsweise die Plattform myclimate.org an.

English Translation:

On 21 January 2020, the D 6 Department of Legal Affairs of the Federal Ministry of the Interior, Building and Community announced as part of an anticipatory arrangement that **with immediate effect, business travelers will be reimbursed the costs of a rail journey on a voluntary basis even if the business trip is more expensive and takes longer than if a flight is used.** This also includes additional overnight and daily allowances.

This is a first step towards implementing point 3.5.1.3 "Reduction of emissions from business travel" contained in the Federal Government's Climate Protection Program 2030. The corresponding extract from the Climate Protection Program is attached.

For new business trips to be applied for, the Travel Agency will not refer to a more economical offer from airlines, provided that the business traveler wishes to use the railways.

Before applying for rail travel as an alternative to flight, the travel procedure at the Institute must be agreed with the respective supervisor. This is especially the case if a significant extension of one to a maximum of two days of the travel time is caused by the use of the railway. In this way, later cancellation costs can be avoided. An extension of the business trip beyond this is no longer justifiable.

All rail tickets booked via ORBS are "green tickets" and therefore do not require any further compensation. Voluntary payments for flight compensation are currently not necessary travel expenses and are therefore not reimbursed.

Voluntary CO2 compensation payments made for travel by private motor vehicle in accordance with § 5 BRKG can be reimbursed with immediate effect as incidental costs in accordance with § 10 BRKG on the basis of a standard compensation within the framework of travel expense accounting. The reimbursement of compensation payments for trips with the company car is excluded. Additional donations over and above the standard calculation are not reimbursed.

The Circular of the Federal Ministry of the Interior must be interpreted in such a way that in all cases it is the employee himself who must arrange for the CO2 compensation, not the travel department. The certificate then received must be submitted together with the travel expense report. This procedure is to be applied for each individual business trip and thus excludes a collective compensation payment (e.g. at the end of the year).

As there is not yet a suitable platform for calculating the necessary regular compensation, the business traveler is free to choose the institution with which they would like to make their compensation payment, for example the myclimate.org platform.

Weitere Informationen / Further Information:

<https://www.bundesregierung.de/breg-de/aktuelles/nachhaltige-mobilitaet-voranbringen-1707928>
<https://www.nature.com/articles/d41586-019-02747-6>
<https://www.horizonte-magazin.ch/2019/03/07/wissenschaft-muss-den-eigenen-co2-ausstoss-drosseln/> (German)
<http://www.russpoldrack.org/2019/06/why-i-will-be-flying-less.html>
<https://noflyclimatesci.org/>

Quellen / Sources:

- [1] https://www.mpimet.mpg.de/fileadmin/download/Grassl_Brockhagen.pdf
- [2] <https://ethz.ch/content/dam/ethz/associates/services/organisation/Schulleitung/mobilitaetsplattform/Factsheet%20air%20travel%20ETH%20Zurich.pdf>
- [3] <https://www.co2online.de/klima-schuetzen/mobilitaet/bahn-oder-flugzeug-der-vergleich/>
- [4] https://www.bahn.de/p/view/bahnbusiness/info/gruene_geschaeftsreisen.shtml
- [5] https://www.gesetze-im-internet.de/brkg_2005/BJNR141810005.html

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316. Sandra Schnädelbach (MPI für Bildungsforschung, Berlin)
317. Christina Leuker (MPI für Bildungsforschung, Berlin)
318. Niels Kloosterman (MPI für Bildungsforschung, Berlin)
319. Susannah Goss (MPI für Bildungsforschung, Berlin)
320. Karsten Lichau (MPI für Bildungsforschung, Berlin)
321. Tina Seemann (MPI für Kolloid- und Grenzflächenforschung, Potsdam)
322. Susanne Schwarz-Esser (MPI für Gesellschaftsforschung, Köln)
323. Corinna Laube (MPI für Bildungsforschung, Berlin)
324. Tim Birkenbach (MPI für Sozialrecht und Sozialpolitik, München)
325. Martin J. Dahl (MPI für Bildungsforschung, Berlin)
326. Mareike Rentzsch (MPI für Kolloid- und Grenzflächenforschung, Potsdam)
327. Kerstin Gabbe (MPI für Kolloid- und Grenzflächenforschung, Potsdam)
328. Mareike Stephan (MPI für Kolloid- und Grenzflächenforschung, Potsdam)
329. Michael Lohaus (MPI für Intelligente Systeme, Tübingen)
330. Stefan Gruber (MPI für Sozialrecht und Sozialpolitik, München)
331. Daniel C. Schneider (MPI für demografische Forschung, Rostock)
332. Luca Salerno (MPI für Sozialrecht und Sozialpolitik, München)
333. Sabrina Zuber (MPI für Sozialrecht und Sozialpolitik, München)
334. Melanie Wagner (MPI für Sozialrecht und Sozialpolitik, München)
335. Kathrin Axt (MPI für Sozialrecht und Sozialpolitik, München)
336. Johannes Rausch (MPI für Sozialrecht und Sozialpolitik, München)
337. Michael Bergmann (MPI für Sozialrecht und Sozialpolitik, München)
338. Sven Roßwog (MPI für Sozialrecht und Sozialpolitik, München)
339. Gregor Sand (MPI für Sozialrecht und Sozialpolitik, München)
340. Johanna Bristle (MPI für Sozialrecht und Sozialpolitik, München)
341. Renate Eggenreich (MPI für Sozialrecht und Sozialpolitik, München)
342. Tessa-Virginia Hannemann (MPI für Sozialrecht und Sozialpolitik, München)
343. David Heller (MPI für molekulare Genetik, Berlin)
344. Elena Sommer (MPI für Sozialrecht und Sozialpolitik, München)
345. Lena Rudeck (MPI für Bildungsforschung, Berlin)
346. Markus Pözlberger (MPI für Quantenoptik, Garching)
347. David Rüll (MPI für Steuerrecht und Öffentliche Finanzen, München)
348. Tim Rohmann (MPI für Sozialrecht und Sozialpolitik, München)
349. Felix Pözl (MPI für Radioastronomie, Bonn)
350. Laila Linke (MPI für Radioastronomie, Bonn)
351. Jörg Burdanowitz (MPI für Meteorologie, Hamburg)
352. Abhijeet Krishna (MPI für molekulare Zellbiologie und Genetik, Dresden)
353. Miriam Liedvogel (MPI für Evolutionsbiologie, Plön)
354. Tobias Lenz (MPI für Evolutionsbiologie, Plön)
355. R. Guy Reeves (MPI für Evolutionsbiologie, Plön)
356. Bernhard Haubold (MPI für Evolutionsbiologie, Plön)
357. Stephanie Stuck (MPI für Sozialrecht und Sozialpolitik, München)
358. Jürgen Schreiber (MPI für Astronomie, Heidelberg)
359. Philipp Kaniuth (MPI für Kognitions- und Neurowissenschaften, Leipzig)
360. Janine Prater (MPI für molekulare Zellbiologie und Genetik, Dresden)
361. Corinna Coupette (MPI für Informatik, Saarbrücken)
362. Jonathan Schindler (MPI für Steuerrecht und Öffentliche Finanzen, München)
363. Luc Desautettes-Barbero (MPI für Innovation und Wettbewerb, München)
364. Philipp Grotkamp (MPI für Innovation und Wettbewerb, München)
365. Franciska Engeser (MPI für Sozialrecht und Sozialpolitik, München)
366. Christoph Lenzen (MPI für Informatik, Saarbrücken)
367. Karl Bringmann (MPI für Informatik, Saarbrücken)
368. Christian Rödenbeck (MPI für Biogeochemie, Jena)
369. Nick Fischer (MPI für Informatik, Saarbrücken)
370. Theresa Fabel (MPI für Sozialrecht und Sozialpolitik, München)
371. Henrik Brumm (MPI für Ornithologie, Seewiesen)
372. Luzia Weiss (MPI für Sozialrecht und Sozialpolitik, München)
373. Soňa Mikulová (MPI für Bildungsforschung, Berlin)

374. Margit Hinkel (MPI für Innovation und Wettbewerb, München)
375. Philip Thomas (MPI für Quantenoptik, Garching)
376. Franziska Müller (MPI für Informatik, Saarbrücken)
377. Martina Oltrogge (MPI für Ornithologie, Seewiesen)
378. Jamal Malik (MPI für Kolloid- und Grenzflächenforschung, Potsdam)
379. Jo Mhairi Hale (MPI für demografische Forschung, Rostock)
380. Tobias Leutritz (MPI für Kognitions- und Neurowissenschaften, Leipzig)
381. Knut Heidemann (MPI für Dynamik und Selbstorganisation, Göttingen)
382. Nicole Lorenz (MPI für Kognitions- und Neurowissenschaften, Leipzig)
383. Mathias Goldau (MPI für Kognitions- und Neurowissenschaften, Leipzig)
384. Joshua Grant (MPI für Kognitions- und Neurowissenschaften, Leipzig)
385. Burkhard Maess (MPI für Kognitions- und Neurowissenschaften, Leipzig)
386. Anna-Lena Tebbe (MPI für Kognitions- und Neurowissenschaften, Leipzig)
387. Regine Schwab (MPI für ethnologische Forschung, Halle (Saale))
388. Alexander von Rohr (MPI für Intelligente Systeme, Stuttgart)
389. Eugen Wassiliwizky (MPI für empirische Ästhetik, Frankfurt am Main)
390. Maria José Mendoza Jiménez (MPI für Sozialrecht und Sozialpolitik, München)
391. Veronika Máté (MPI für Sozialrecht und Sozialpolitik, München)
392. Alexander Schumacher (MPI für Sozialrecht und Sozialpolitik, München)
393. Melissa Pflüger (MPI für Sozialrecht und Sozialpolitik, München)
394. Nicolas Goll (MPI für Sozialrecht und Sozialpolitik, München)
395. May Khourshed (MPI für Sozialrecht und Sozialpolitik, München)
396. Xiangchun Ju (MPI für evolutionäre Anthropologie, Leipzig)
397. Wulf Hevers (MPI für evolutionäre Anthropologie, Leipzig)
398. Julia Wambach (MPI für Bildungsforschung, Berlin)
399. Lieneke Janssen (MPI für Kognitions- und Neurowissenschaften, Leipzig)
400. Caroline Glenk (MPI für Steuerrecht und Öffentliche Finanzen, München)
401. Sarah Collet (MPI für Steuerrecht und Öffentliche Finanzen, München)
402. Karin Schuller (MPI für Sozialrecht und Sozialpolitik, München)
403. Núria Muñoz Garganté (MPI für Wissenschaftsgeschichte, Berlin)
404. Rocco Gaudenzi (MPI für Wissenschaftsgeschichte, Berlin)
405. Judith Kronschnabl (MPI für Sozialrecht und Sozialpolitik, München)
406. Alexander von Schwerin (MPI für Wissenschaftsgeschichte, Berlin)
407. Beatrix Fauler (MPI für molekulare Genetik, Berlin)
408. Elisabeth Jostock (MPG Generalverwaltung, München)
409. Christoph Rosol (MPI für Wissenschaftsgeschichte, Berlin)
410. Walburga Pfündl (MPG Generalverwaltung, München)
411. Sandra Martin (MPI für Kognitions- und Neurowissenschaften, Leipzig)
412. Elena Essel (MPI für evolutionäre Anthropologie, Leipzig)
413. Marianna Szczygielska (MPI für Wissenschaftsgeschichte, Berlin)
414. Zoé Rehder (MPI für Meteorologie, Hamburg)
415. Tobias Becker (MPI für Meteorologie, Hamburg)
416. Dirk Olonscheck (MPI für Meteorologie, Hamburg)
417. Rene Redler (MPI für Meteorologie, Hamburg)
418. Carola Kauhs (MPI für Meteorologie, Hamburg)
419. Hongmei Li (MPI für Meteorologie, Hamburg)
420. István Dunkl (MPI für Meteorologie, Hamburg)
421. Edda Einfeldt (MPI für molekulare Genetik, Berlin)
422. Veronika Gayler (MPI für Meteorologie, Hamburg)
423. Antje Weitz (MPI für Meteorologie, Hamburg)
424. Jeremy C. Rugenstein (MPI für Meteorologie, Hamburg)
425. Jörn Heinemeier (MPI für Meteorologie, Hamburg)
426. Thomas Raddatz (MPI für Meteorologie, Hamburg)
427. Jonas Klee (MPI für ethnologische Forschung, Halle (Saale))
428. Michaela Born (MPI für Meteorologie, Hamburg)
429. Aaron Spring (MPI für Meteorologie, Hamburg)
430. Ksenia Kuznetsova (MPI für molekulare Zellbiologie und Genetik, Dresden)
431. Flavio D'Abramo (MPI für Wissenschaftsgeschichte, Berlin)
432. Barbara Borgonovo (MPI für molekulare Zellbiologie und Genetik, Dresden)
433. Stephan Janosch (MPI für molekulare Zellbiologie und Genetik, Dresden)
434. Robert Arnes (MPI für molekulare Zellbiologie und Genetik, Dresden)
435. Cordula Andree (MPI für molekulare Zellbiologie und Genetik, Dresden)
436. Kirsten Kelleher (MPI für molekulare Genetik, Berlin)
437. Martin Küblbeck (MPI für Ornithologie, Seewiesen)
438. Margherita Cragnolini (MPI für Ornithologie, Seewiesen)
439. Mäggi Hieber Ruiz (MPI für Verhaltensbiologie, Radolfzell)

- 440. Hemal Naik (MPI für Verhaltensbiologie, Radolfzell)
- 441. Karl-Ernst Kaissling (MPI für Ornithologie, Seewiesen)
- 442. Lara Keicher (MPI für Verhaltensbiologie, Radolfzell)
- 443. Robert Kraus (MPI für Verhaltensbiologie, Radolfzell)
- 444. Dina Dechmann (MPI für Verhaltensbiologie, Radolfzell)
- 445. Fabian Heim (MPI für Ornithologie, Seewiesen)
- 446. Agnes Türk (MPI für Ornithologie, Seewiesen)
- 447. Nelly Helmbrecht (MPI für evolutionäre Anthropologie, Leipzig)
- 448. Stefania Casagrande (MPI für Ornithologie, Seewiesen)
- 449. Marco Kleine (MPI für Innovation und Wettbewerb, München)
- 450. Lotte Schlicht (MPI für Ornithologie, Seewiesen)
- 451. Ulf Schroeder (MPI für molekulare Genetik, Berlin)
- 452. Zozan Comak (MPI für molekulare Genetik, Berlin)
- 453. Johannes Zierenberg (MPI für Dynamik und Selbstorganisation, Göttingen)
- 454. Daniela Hellwig (MPI für Plasmaphysik, Garching)
- 455. Michael Erdmann (MPI für Plasmaphysik, Garching)
- 456. Edda Einfeldt (MPI für molekulare Genetik, Berlin)
- 457. Mariella Paul (MPI für Kognitions- und Neurowissenschaften, Leipzig)
- 458. Arno Villringer (MPI für Kognitions- und Neurowissenschaften, Leipzig)
- 459. Anagha Deshmane (MPI für biologische Kybernetik, Tübingen)
- 460. Charlotte Scheinpflug (MPI für Neurobiologie, Martinsried)
- 461. Petra Jahn (MPI für evolutionäre Anthropologie, Leipzig)
- 462. Petra Küchenmeister (MPI für Gesellschaftsforschung, Köln)
- 463. Viola Priesemann (MPI für Dynamik und Selbstorganisation, Göttingen)
- 464. Friedhelm Jansen (MPI für Meteorologie, Hamburg)
- 465. Christine Gieraths (MPG Generalverwaltung, München)
- 466. Stefan Fabry (MPG Generalverwaltung, München)
- 467. Sandra Wirkner (MPG Generalverwaltung, München)
- 468. Petra Kamm (MPG Generalverwaltung, München)
- 469. Roland Kniebühler (MPG Generalverwaltung, München)
- 470. Susanne Uebele (Archiv der MPG, Berlin)
- 471. Heinrich Widmann (Deutsches Klimarechenzentrum, Hamburg)
- 472. Michaela Hergersberg (MPG Generalverwaltung, München)
- 473. Isabel Beeg (MPG Generalverwaltung, München)
- 474. Barbara Müller (MPG Generalverwaltung, München)
- 475. Kristin Münch (MPG Generalverwaltung, München)
- 476. Ralph Ernstorfer (Fritz-Haber-Institut der MPG, Berlin)
- 477. Maria Eichinger-Kiermeier (MPG Generalverwaltung, München)
- 478. Michael Nagel (MPG Generalverwaltung, München)
- 479. Stefanie Dedek (MPG Generalverwaltung, München)
- 480. Vivek Devulapalli (MPI für Eisenforschung, Düsseldorf)
- 481. Susan Hachgenei (MPG Generalverwaltung, München)
- 482. Katrin Matthes (MPI für Marine Mikrobiologie, Bremen)

A2.10 “Kompensation von CO₂-Emissionen durch Reiseaktivitäten in der Max-Planck-Gesellschaft”

Kompensation von CO₂-Emissionen durch Reiseaktivitäten in der Max-Planck-Gesellschaft

Positionspapier der Arbeitsgruppe "CO₂-Kompensation" des Max-Planck-Nachhaltigkeits-Netzwerkes

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Zusammenfassung

Wir fordern die Max-Planck-Gesellschaft (MPG) auf, die Anzahl der Flugreisen zu reduzieren und eine entsprechende Verhaltensänderung ihrer Wissenschaftler*innen und Mitarbeiter*innen zu fördern, aber auch die mit unvermeidlichen Flugreisen verbundenen CO₂-Emissionen zu kompensieren. Wir schlagen vor, dass die MPG die offizielle Erlaubnis, Fördermittel für solche Kompensationen zu verwenden, bei der Gemeinsamen Wissenschaftskonferenz (GWK) als Zuwendungsgeber einholt. Um dieses Anliegen in der GWK zu thematisieren, bitten wir die MPG, sich in der Allianz der Wissenschaftsorganisationen (Allianz) für die Möglichkeit der CO₂-Kompensation einzusetzen. Bei Bedarf sollte die MPG innerhalb der Allianz die Führungsrolle hierfür übernehmen. Nach erfolgter Erlaubnis durch die GWK sollte die MPG ein verbindliches CO₂-Kompensationssystem für alle Max-Planck-Institute (MPI) einführen. Kompensationsgebühren sollten dabei nicht durch zentrale Mittel der MPG, sondern aus den Institutsbudgets abgedeckt werden, um einen Anreiz zur Änderung des Reiseverhaltens zu schaffen. Die MPG sollte verschiedene Optionen zur CO₂-Kompensation prüfen und umgesetzte Konzepte kontinuierlich evaluieren, um die Option mit dem größten ökologischen Nutzen zu identifizieren. Um unmittelbar aktiv zu werden, schlagen wir eine sofortige Umsetzung einer Pilotphase der "externen" Kompensation in Kooperation mit Nichtregierungsorganisationen (NGO) wie atmosfair, PrimaKlima etc. vor.

Einführung

Der Klimawandel ist eine der größten Herausforderungen unserer Zeit. Durch ihre Arbeit erforschen Wissenschaftler*innen die Ursachen des Klimawandels und tragen dazu bei, Lösungen für den Klimaschutz zu entwickeln und das Bewusstsein für dieses Thema zu schärfen. Gleichzeitig haben Wissenschaftler*innen durch ihre Forschungsarbeit auch ihren Anteil an den globalen CO₂-Emissionen. Wir wollen die durch die Wissenschaft verursachten CO₂-Emissionen reduzieren, ohne die Freiheit der Wissenschaft zu beeinträchtigen. Ein wesentlicher Anteil der CO₂-Emissionen in Wissenschaft und Forschung ist auf die Reisetätigkeit von Wissenschaftler*innen im Luftverkehr zurückzuführen. Derzeit liegen uns keine belastbaren Zahlen über den CO₂-Ausstoß durch Reisetätigkeiten von Wissenschaftler*innen im Allgemeinen vor. Eine Studie der ETH Zürich ergab, dass rund 55% ihrer gesamten CO₂-Emissionen auf die Flugreisen ihrer Wissenschaftler*innen zurückzuführen ist. Es ist anzunehmen, dass der Anteil der Flugreisen an den Gesamtemissionen von CO₂ in anderen Wissenschaftsorganisationen wie der MPG ähnlich hoch ist. Um die durch die Wissenschaft verursachten CO₂-Emissionen zu reduzieren, ist es daher nur konsequent, primär das Thema Flugreisen anzugehen. Gleichzeitig wollen wir den wissenschaftlichen Austausch weltweit aufrechterhalten bzw. intensivieren. Mit diesem Positionspapier möchten wir eine Strategie zur Reduzierung und Kompensation der CO₂-Emissionen durch Flugreisen in der MPG vorschlagen.

Reduktion der CO₂-Emissionen durch Flugreisen

Wir schlagen eine dreistufige Strategie vor, um CO₂-Emissionen durch Flugreisen in der MPG zu reduzieren:

1. **Vermeidung** von Dienstreisen, die nicht absolut notwendig sind, und Substitution durch alternative Methoden des wissenschaftlichen Austausches, wie z.B. durch den verstärkten Einsatz von Videokonferenzen
2. **Reduktion** der CO₂-Emissionen durch eine entsprechende Wahl der Verkehrsmittel: Zug statt Flug, Auswahl von effizienteren Flugzeugen, Economy- statt Business-Klasse, direkte Flüge etc.
3. **Kompensation** der CO₂-Emissionen für unvermeidbare Flugreisen

Die Reihenfolge der Stufen entspricht auch unserer Prioritätensetzung. In diesem Positionspapier befassen wir uns mit den Möglichkeiten der Kompensation von CO₂-Emissionen (Stufe 3). Konzepte für Stufen 1 und 2 werden von entsprechenden Arbeitsgruppen des Max-Planck-Nachhaltigkeits-Netzwerkes ausgearbeitet.

Konzepte der CO₂-Kompensation

Das grundlegende Konzept der CO₂-Kompensation basiert auf zwei Prinzipien:

Ausgleich: Für jeden Flug wird der mutmaßliche Anteil an CO₂-Emissionen berechnet und die Kosten entsprechender Ausgleichsmaßnahmen abgeschätzt. Typische Ausgleichsmaßnahmen sind zum Beispiel Wiederaufforstung oder die Investitionen in Technologien zur Reduktion von CO₂ an anderer Stelle. Die Kompensationsgebühr wird dann für eben solche Maßnahmen eingesetzt. Wesentlich ist dabei, dass die durch Kompensationsgebühren zur Verfügung stehenden finanziellen Ressourcen ausschließlich für Projekte eingesetzt werden, die ohne diese Kompensationsmittel nicht umgesetzt werden würden.

Nudging (Anreizsystem): Kompensationsgebühren sollen ein klimafreundlicheres Reiseverhalten motivieren. Dies geschieht einerseits dadurch, dass die durch die Kompensationsgebühren erhöhten Kosten einer Reise, z.B. mit dem Flugzeug, den einhergehenden Klimaschaden besser illustrieren. Weiterhin soll die Möglichkeit, Kompensationsgebühren durch klimafreundliches Reisen zu vermeiden, ein Anreiz für eine Verhaltensänderung sein, auch wenn die für die Reise verantwortlichen Personen oder Einrichtungen aus Gründen des reinen Klimaschutzes hierzu keine Veranlassung sehen. Daher sollten die Kompensationsgebühren nicht von einer zentralen Stelle bezahlt werden, sondern aus den Budgets der Personen oder Einrichtungen, die für die Reise verantwortlich sind. Ebenso ist es wichtig, dass bei einem Kostenvergleich zwischen Flugreise und klimafreundlicheren Alternativen für eine Reisebuchung die Kompensationsgebühren für die Flugreise mit einbezogen werden.

Sollte ein Kompensationskonzept in der MPG umgesetzt werden, ist darauf zu achten, dass Kompensationsgebühren aus den Institutshaushalten entnommen werden und nicht aus einem gemeinsamen MPG-weiten Topf. Institutsverwaltungen können oder sollen die Kompensationskosten entsprechend der Reiseaktivität auf die verschiedenen Institutsabteilungen verteilen.

Wir sind der Meinung, dass ein wirksames Kompensationskonzept folgende Anforderung erfüllen sollte:

- **Effektiv** als Anreizsystem ("Nudging")
- **Effizient** im Sinne des CO₂-Ausgleichs
- **Umsetzbar** im Sinne des Verwaltungsaufwandes
- **Transparent** innerhalb der MPG und für die Öffentlichkeit

Unabhängig davon, für welches Konzept sich die MPG entscheidet, ist es wichtig, dass die Erfüllung der vier Anforderungen regelmäßig evaluiert wird.

Zur Kompensation von CO₂-Emissionen gibt es verschiedene Konzepte, die die vier Anforderungen unserer Meinung nach in unterschiedlichem Maße erfüllen, und im Folgenden kurz erläutert werden sollen.

Externe CO₂-Kompensation

Das am meisten verbreitete Konzept zur Kompensation von CO₂ - insbesondere von CO₂-Emissionen durch Reisetätigkeiten - besteht in Abgaben (Spenden) an NGOs, z.B. atmosfair oder PrimaKlima, die die Mittel für Maßnahmen zum Ausgleich der CO₂-Emissionen verwenden.^{1,2} Die NGOs evaluieren die geförderten Klimaschutzprojekte und werden selbst durch unabhängige nationale Institutionen, z.B. dem TÜV Rheinland³, oder durch internationale Institutionen der UN-Klimaschutzbehörde UNFCCC⁴ zertifiziert. Dabei werden Zertifikate mit unterschiedlichen CO₂-Kompensationseffizienzen vergeben. Die meisten NGOs für CO₂-Kompensation bieten auch an, dass die kompensierenden Einrichtungen Projekte auswählen können, für die Mittel bereitgestellt werden sollen. Da es sich bei der Entschädigungsgebühr rechtlich um eine Spende handelt, können die Kompensationsgebühren steuerlich geltend gemacht werden.

Ein solches Konzept der CO₂-Kompensation wird bisher vor allem von Privatpersonen oder Unternehmen angewendet. In jüngster Zeit nutzen jedoch auch öffentliche Einrichtungen, darunter wenige wissenschaftliche Einrichtungen, die CO₂-Kompensation für Flugreisen. Dazu gehören z.B.:

- Bundeskanzleramt, Bundestag, alle Bundesministerien und Bundesbehörden⁵
- Alfred-Wegner-Institut, Bremerhaven⁶
- Helmholtz-Zentrum für Umweltforschung⁷
- Öko-Institut e.V.⁸
- Eidgenössische Technische Hochschule Zürich⁹
- Landeshauptstadt München¹⁰
- Freie Hansestadt Hamburg¹¹

Aufgrund rechtlicher Beschränkungen im Zuwendungsrecht, ist es öffentlichen Forschungseinrichtungen derzeit nicht gestattet, Kompensationszahlungen für CO₂-Emissionen zu leisten. Um CO₂-Kompensationen für öffentlich geförderte Forschungseinrichtungen möglich zu machen, ist es notwendig, dass die GWK diese erlaubt.

¹ <https://www.umweltbundesamt.de/themen/freiwillige-co2-kompensation> , 08.11.2019

² <https://www.zeit.de/die-antwort/2019-06/co2-kompensation-klimabilanz-fluege-faq#ist-kompensieren-sinnvoll> , 08.11.2019

³ https://www.atmosfair.de/wp-content/uploads/JB_2015.pdf , 08.11.2019

⁴ <https://unfccc.int/process-and-meetings/the-kyoto-protocol/mechanisms-under-the-kyoto-protocol/the-clean-development-mechanism> , 08.11.2019

⁵ <https://www.umweltbundesamt.de/presse/pressemittelungen/bundesregierung-kompensiert-alle> , 08.11.2019

⁶ <https://www.awi.de/ueber-uns/organisation/nachhaltigkeit/co2-kompensation-fuer-dienstreisen.html> , 08.11.2019

⁷ https://www.ufz.de/export/data/2/233071_umwelterklaerung2018.pdf , 08.11.2019

⁸ <https://www.oeko.de/aktuelles/2016/kompensation-von-treibhausgasemissionen-am-oeko-institut/> , 08.11.2019

⁹ <https://www.ethz.ch/services/de/finanzen-und-controlling/ethis/ethis-help/flugreisen.html> , 08.11.2019

¹⁰ https://www.muenchen.de/rathaus/Stadtverwaltung/Referat-fuer-Gesundheit-undUmwelt/Klimaschutz_und_Energie/Atmosfair.html , 08.11.2019

¹¹ <https://www.atmosfair.de/de/klimaschutzprojekte/biogas-biomasse/tanzania-composting-facility-fororganic-market-waste/> 08.11.2019

Vor- und Nachteile der "externen" Kompensationen lassen sich unserer Meinung nach wie folgt zusammenfassen:

Vorteile:

- **Effektiv** als Anreiz, da die finanziellen Mittel dem Institut nicht mehr zur Verfügung stehen
- Leichte **Umsetzbarkeit**, da entsprechende Verfahren sehr gut entwickelt und in anderen öffentlichen Einrichtungen bereits etabliert sind
- Geringer Evaluierungsaufwand für die kompensierenden Institute
- **Transparent**, da bekanntes Konzept, insbesondere für die Öffentlichkeit
- Allgemein anerkanntes Konzept der CO₂-Kompensation

Nachteile:

- **Effizienz** der Kompensationsmaßnahmen wird teilweise in Frage gestellt¹²
- **Umsetzbarkeit** anfangs eingeschränkt durch die rechtlichen Bestimmungen des aktuellen Zuwendungsrechts (Erlaubnis der GWK erforderlich)
- Finanzielle Mittel sind für die kompensierenden Institute „verloren“
- Eingeschränkte Auswahl der Kompensationsprojekte

Interne CO₂-Kompensation

Als alternative oder ergänzende Maßnahme zur Bereitstellung von Mitteln für NGOs ("externe Kompensation") könnten „interne“ CO₂-Kompensationskonzepte in Betracht gezogen werden, bei denen zwar Kompensationsgebühren erhoben werden, die finanziellen Mittel aber innerhalb der MPG verbleiben und intern für Ausgleichsmaßnahmen eingesetzt werden. Die Effizienz der Ausgleichsmaßnahmen könnte dabei theoretisch höher als bei der externen Kompensation aber auch niedriger sein; weitere Forschung ist erforderlich, um hierfür effiziente Verfahren zu entwickeln und zu bewerten. Für die interne Kompensation gibt es verschiedene Optionen. Diese haben folgende Vor- und Nachteile gemeinsam:

Vorteile:

- Die finanziellen Mittel verbleiben innerhalb der MPG/Institute
- Möglicherweise größere Auswahl bei der Verteilung der Mittel aus den Kompensationsgebühren auf verschiedene Projekte

Nachteile:

- **Effizienz** der Kompensationsmaßnahme muss durch die MPG selbst evaluiert werden
- Geringerer **Anreizeffekt**, da der MPG keine Mittel verloren gehen und somit weniger Anreiz zu klimafreundlichen Reisen besteht
- Schwerfälligere **Umsetzbarkeit** aufgrund eines erhöhten Verwaltungsaufwandes
- Kompensationsgebühren werden möglicherweise für Maßnahmen eingesetzt, die auch ohne Kompensationskonzept durchgeführt werden würden

Für das Konzept der internen Kompensation haben wir drei wesentliche Optionen identifiziert, die im Folgenden erläutert werden sollen.

¹² https://ec.europa.eu/clima/sites/clima/files/ets/docs/clean_dev_mechanism_en.pdf , 08.11.2019

Ausgleichsmaßnahmen

Die durch eine interne CO₂-Kompensationsgebühr gesammelten Mittel könnten in Maßnahmen zur Reduzierung der CO₂-Emissionen innerhalb der MPG investiert werden, wie z.B. der Modernisierung der Gebäudeisolierung, der Installation von Photovoltaik-Kraftwerken, den Kauf von energieeinsparenden Geräten etc. Eine solche Maßnahme hat jedoch keine Wirkung, wenn diese auch ohne die Kompensationsgebühr umgesetzt werden würde. Wenn beispielsweise ein altes Forschungsgebäude saniert werden muss und ohnehin eine Erneuerung der Isolierung geplant ist, dann ist es nicht sinnvoll, für diese Maßnahme Mittel aus einem CO₂-Kompensationskonzept einzusetzen. Jede CO₂-Reduktionsmaßnahme durch ein Kompensationskonzept sollte ein zusätzlicher Aufwand sein, um eine wirklich ausgleichende Wirkung zu erzielen.

Vorteile & Nachteile: siehe allgemeine Vor- und Nachteile der internen Kompensation

Subvention von klimafreundlichen Reisen

Klimafreundlichere Verkehrsmittel wie Züge sind oft teurer als Flugreisen. Mit Mitteln aus einer internen Ausgleichsgebühr könnten ökologischere Verkehrsmittel wie Bahnreisen gefördert werden.

Vorteile:

- Hoher **Anreizeffekt**, nachvollziehbarer Zusammenhang zwischen Kompensationsgebühr und -maßnahme, Motivation zur Dienstreisen mit kürzeren Strecken
- Hohe **Effizienz** der CO₂-Kompensationsmaßnahme
- Hohe **Transparenz**
- Verbessert die Reisemöglichkeiten in Europa für Promovierende und Postdoktorand*innen mit geringem Reisebudget

Nachteile:

- Umverteilung der Kompensationsgebühren zur Subvention von klimafreundlichen Reisen muss erst entwickelt und organisiert werden (**Umsetzbarkeit**)
- Möglicher Rebound-**Effekt**, erhöhte regionale Reiseaktivität, evtl. auch von nicht notwendigen Reisen

Investition in Nachhaltigkeitsforschung

Mittel aus einer internen Kompensationsgebühr könnten für die Forschung in der MPG zum Thema Klimawandel und Klimaschutz bereitgestellt werden. Ein solches Konzept (CO₂MPASS) wurde von Tobias Erb (MPI-TM Marburg) und Eberhard Bodenschatz (MPI-DS Göttingen) vorgeschlagen.

Vorteile:

- Mittel werden für den eigentlichen Zweck der MPG verwendet (Grundlagenforschung)

Nachteile:

- Möglicherweise schwierige **Umsetzbarkeit** bei der Verteilung der Mittel
- **Effizienz** der CO₂-Kompensation schwierig zu evaluieren
- Umgekehrter **Anreizeffekt**: je mehr geflogen wird, umso mehr wird in die Nachhaltigkeitsforschung investiert
- Risiko ungenutzter Mittel oder Senkung des wissenschaftlichen Standards, falls nicht genügend oder keine qualifizierten Projekte der Nachhaltigkeitsforschung im Rahmen des Kompensationskonzeptes vorgeschlagen werden

Rechtliche Aspekte

Bundesreisekostengesetz

Unserem Kenntnisstand nach gibt es im Bundesreisekostengesetz (BRKG) keine Regelungen, die dem Konzept der CO₂-Kompensation explizit widersprechen würden. Obwohl die CO₂-Kompensationsgebühren mit einer bestimmten Reisetätigkeit zusammenhängen, sind sie nicht Teil der direkten und offiziellen Reisekosten. Aus diesem Grund berührt das BRKG nicht den Aspekt der CO₂-Kompensation. Einige Transportunternehmen wie Fluggesellschaften, Busunternehmen usw. bieten die CO₂-Kompensation als Teil des Tickets an. In diesem Fall könnten die zusätzlichen Kosten ein Problem für das BRKG und weitere rechtliche Klarstellungen erforderlich sein.

Zuwendungsrecht

Unserem Kenntnisstand nach gibt es seitens des Zuwendungsrecht keine rechtlichen Einwände gegen das Konzept der internen CO₂-Kompensation, da die Mittel beim Zuwendungsempfänger verbleiben und dort nach Zuwendungsrecht eingesetzt werden. Alle Maßnahmen der entsprechenden Kompensationskonzepte wie z.B. Investitionen in die Nachhaltigkeitsforschung, eine Umverteilung von Mitteln innerhalb der Reisebudgets zugunsten klimafreundlicher Verkehrsmittel oder die energetische Sanierung von Forschungsgebäuden sind im Einklang mit dem Zuwendungsrecht, da diese Maßnahmen unmittelbar den Forschungsaufgaben und dem Wissenschaftsbetrieb dienen. Im Gegensatz dazu hat die MPG derzeit keine rechtlichen Möglichkeiten, öffentliche Gelder für Konzepte der externen CO₂-Kompensation zu verausgaben. Sollen externe CO₂-Kompensationen in der MPG umgesetzt werden, so muss dies von der GWK, die für alle Forschungseinrichtungen zuständig ist, die aus Bundes- und Landesmitteln finanziert werden, ausdrücklich genehmigt werden.

Schlussfolgerungen

CO₂-Emissionen in Wissenschaft und Forschung werden ein immer wichtigeres Thema, insbesondere vor dem Hintergrund der aktuellen gesellschaftlichen Debatten. Wir glauben, dass sich die Max-Planck-Gesellschaft dieser Herausforderung stellen und geeignete Ansätze entwickeln sollte, um die CO₂-Emissionen, insbesondere durch Reisetätigkeiten, zu reduzieren. Dem Problem der CO₂-Emissionen durch Reiseaktivitäten sollte in erster Linie begegnet werden, indem die Anzahl der Reisen verringert und klimafreundlicheren Verkehrsmitteln Vorrang eingeräumt wird. Im Falle unvermeidbarer Flugreisen sollten die CO₂-Emissionen von den für die CO₂-Emissionen verursachenden Instituten kompensiert werden. Verschiedene Konzepte zur Kompensation von CO₂-Emissionen können in „externe“ und „interne“ Konzepte unterteilt werden. Welches Konzept für die Max-Planck-Gesellschaft am besten geeignet ist, muss sorgfältig geprüft werden. In der Zwischenzeit schlagen wir vor, dass die MPG während einer Pilotphase eine externe Kompensation in Kooperation mit NGOs für CO₂-Kompensation testet. Die externe Kompensation zeichnet sich durch hohe Anzeizeffekte, hohe Transparenz innerhalb der MPG und für die Öffentlichkeit sowie geringen Verwaltungsaufwand aus. Die Effizienz der externen CO₂-Kompensation ist derzeit teilweise umstritten und sollte von der MPG, vorzugsweise durch ein entsprechendes Forschungsprojekt, überwacht werden. Um eine externe CO₂-Kompensation zu ermöglichen, wird die MPG aufgefordert, hierfür die Erlaubnis bei der GWK einzuholen. Zu diesem Zweck sollte sich die MPG für die Möglichkeit der CO₂-Kompensation innerhalb der Allianz der Wissenschaftsorganisationen proaktiv einsetzen. Während der Pilotphase der externen Kompensation soll die Effizienz der externen Kompensation und alternativer Konzepte, insbesondere der oben genannten Ansätze zur internen Kompensation, weiter untersucht werden.

**A2.11 “Kritischer Kommentar zum vorliegenden Fachbeitrag
„Fachbeitrag Wasserrahmenrichtlinie für den Neubau der A 49 im
Abschnitt Stadtallendorf – Gemünden (VKE 40)“ von der ahu GmbH
vom 28.09.2020.”**

Kritischer Kommentar zum vorliegenden Fachbeitrag „Fachbeitrag Wasserrahmenrichtlinie für den Neubau der A 49 im Abschnitt Stadtallendorf – Gemünden (VKE 40)“ von der ahu GmbH vom 28.09.2020.

Am 28.9.2020 wurde ein Fachbeitrag der ahu GmbH mit dem Namen „Fachbeitrag Wasserrahmenrichtlinie für den Neubau der A 49 im Abschnitt Stadtallendorf – Gemünden (VKE 40)“ veröffentlicht. Der Fachbeitrag wurde am 9.7.2020 von der DEGES Deutsche Einheit Fernstraßenplanungs- und -bau GmbH (im Folgenden: DEGES) in Auftrag gegeben. Der Fachbeitrag behandelt maßgeblich die Stellung des Bauvorhabens der A49 durch ein Trinkwasserschutzgebiet in Bezug auf die Europäische Wasserrahmenrichtlinie (WRRL), welches durch die DEGES umgesetzt werden soll. Die gesammelten Kritikpunkte sind im Folgenden zusammengefasst.

In Position 4.1.2 (S. 24-25) diskutieren die Autor*innen die Datenlücken des Fachbeitrages. Sie kommen zu dem Schluss: „Datenlücken im Hinblick auf die WRRL-relevanten Daten und Planunterlagen für das zu bewertende Vorhaben existieren nicht.“ Dieser Aussage wird widersprochen:

In Position 2.2, Unterpunkt „Bauphase“ (S. 14) werden Kontaminationen des Bodens mit Schwermetallen und Sprengstoff diskutiert, für welche die Etablierung eines Bodenmanagements als Maßnahme in der Planfeststellung enthalten bzw. festgeschrieben sei. Für die Einschätzung des Einflusses der Baumaßnahmen auf den chemischen Zustand der betroffenen Wasserkörper ist eine detaillierte Auseinandersetzung mit den dort angesprochenen bestehenden, als heterogen einzuschätzenden Bodenkontaminationen unerlässlich. Speziell durch die besondere Art des jüngst erfolgten und – nach Aussage der Betreibenden – äußerst sensiblen Altlasten-Managements direkt am Grundwasserkörper (GWK) durch Schluck- und Einspeisebrunnen bedarf es für eine abschließende fachliche Bewertung einer konsequenten Offenlegung der aktuellen Datenlage sowie einer detaillierten und kritischen Auseinandersetzung hiermit. Im vorliegenden Fachbeitrag fehlt sie gänzlich.

Angesichts der gegenwärtigen Verschiebung der Niederschlagsintensitäten vom Sommer in den Winter [1], erhöhter Frequenz und Intensität von Überflutungen und Trockenperioden [2] und die damit verbundene natürliche Minderung der Aufnahmekapazität von Wasser in Böden [3,4], ist die Berücksichtigung von aktuellen klimarelevanten Daten grundlegend für die vorgenommene Bewertung sowie die Anpassungen der Bewirtschaftungsziele GWK für den Bewirtschaftungsplan 2022-2027.

Die Situation um die Einleitestelle der Fernableitung in die Klein ist klarzustellen. So ist explizit darzulegen, auf welcher sachlichen Grundlage der Forderung des Zweckverbands Mittelhessischer Wasserversorger (ZMW), die Einleitestelle der Fernableitung

gemäß Wasserschutzgebietsverordnung außerhalb der Wasserschutzzonen II und III A zu verlegen [5], auch in der aktualisierten Planung (vgl. Pos. 1.3, S. 10) nicht nachgekommen wurde. Ebenso ist der endgültige Schluss in Position 5.5, Unterpunkt „Bewertung ökologischer Zustand“, die ökologischen und chemischen Zustände würden durch den Ablauf der Fernableitung nicht beeinflusst, anhand der vorliegenden Daten nicht nachzuvollziehen.

Der in Position 4.1.2 (S. 25) erwähnten Mitteilung der Wasserbehörde (RP Gießen) am 08.09.2020 an DEGES, mit der Aussage, die Verwendung der einzig verfügbaren Messstelle 223 für die Bewertung des chemischen Zustandes der Klein sei fachlich vertretbar (im vorliegenden Fachbeitrag ebenfalls zwingend im Konjunktiv zu formulieren), kann aus wissenschaftlicher Perspektive nicht zugestimmt werden. Die Bewertung des chemischen Zustands eines Gewässers anhand begrenzter Datensätze, erhoben an einem einzelnen Messpunkt außerhalb des zu untersuchenden Gewässers, ist wissenschaftlich nicht tragbar. Das Fehlen von Referenzwerten mindert die Aussagekraft hinsichtlich einer im WRRL Fachbeitrag genannten umfangreichen Datengrundlage massiv; für eine belastbare Interpretation der Daten sind Messungen im diskutierten Gewässer unabdingbar.

Die Diskussion über die Kompensation der wegfallenden Wasserförderung aus den Brunnen des ZMW, die im Rahmen der Bauarbeiten zeitweise außer Betrieb genommen werden müssen (In Pos. 2.2, Unterpunkt „Bauphase“, S. 15 wird der FB28 explizit genannt), fehlt ebenso vollständig. Dies wird als besonders kritisch angesehen, da die Förderkapazitäten des ZMW am GWK nach eigenen Angaben nahezu ausgelastet sind. Eine vollständige Diskussion sollte die durch die für den Bau notwendige geografische Verlagerung der Förderung entstehenden Einflüsse auf den GWK (mit besonderer Berücksichtigung der Altlasten) sowie auf das pflanzenverfügbare Grundwasser ebenso einbeziehen wie die geplante Fördermengensteigerung und den Einfluss der oben diskutierten klimatischen Veränderungen speziell auf die Verlagerung.

Weitere Informationen werden an den folgenden Punkten benötigt:

- In Pos. 5.6.1 (S. 75) wird die Potentialumkehr zwischen Oberflächengewässer und Auengrundwasserleiter kurz angesprochen. Wie zu dem Schluss gekommen wird, dass der chemische Zustand hiervon nicht beeinflusst wird, ist anhand der vorliegenden Information nicht nachzuvollziehen.
- Die kritische Auseinandersetzung mit dem Einbringen von Brückenpfeilern in tiefere Bodenschichten und dem daraus resultierenden Eingriff in die Wasserschutzzone ist im vorliegenden Fachbeitrag ebenfalls nicht aufzufinden.
- Im Allgemeinen und besonders in Pos. 5.5 (S. 71) werden zur Abschätzung der Auswirkungen auf die Qualitätskomponenten der Oberflächenwasserkörper ausschließlich die Oberflächengewässer berücksichtigt. Die Vernachlässigung des oberflächennahen pflanzenverfügbaren Bodenwassers ist nicht begründet.

- Ebenfalls fehlt die Auseinandersetzung mit den anlagebedingten Auswirkungen auf den mengenmäßigen Zustand (Pos. 5.6.2, S. 75-76) im Bereich direkt um die Anlage. Besonders für eine Abschätzung der ökologischen Risiken (durch Verlust an pflanzenverfügbarem Grundwasser) wird diese als notwendig erachtet.
- Eine Auseinandersetzung mit dem Einfluss des Bauvorhabens auf den Wasserhaushalt der Wälder, die durch den Autobahnbau beeinträchtigt werden, fehlt ebenfalls vollständig. Da Wälder im Allgemeinen als wichtige Wasserspeicher und -verdunster fungieren und damit einen direkten Einfluss auf die klimatische Entwicklung der Region haben, würde von einem umfassenden Fachbeitrag eine Berücksichtigung einer entsprechenden Analyse erwartet.

Die folgenden Punkte sind weiterhin zu bemängeln:

- Die Relevanzeinschätzungen „keine Relevanz“ in Tab. 19 sind vielfach nur unter der Annahme gültig, dass alle Auflagen jederzeit vollständig erfüllt werden. Entsprechend ist den Einschätzungen „bei Einhalten und nachweislicher Kontrolle aller Auflagen“ hinzuzufügen und entsprechende Kontroll-, Vorsichts- und Präventivmaßnahmen explizit zu diskutieren und zu realisieren.
- Der Relevanzeinschätzung in der Spalte „Erschütterungen“ in Tab. 19 (S. 50 – „keine Relevanz“) wird gänzlich widersprochen. Die Annahme, dass die Einhaltung aller vorhandener Auflagen – die einer eigenen Risikostudie der ahu GmbH zugrunde liegen – jegliche – besonders für den Zustand des Wassers – problematische Erschütterungen vermeide, ist grob vereinfacht und besonders mit Blick auf die geplanten Tunnelbohrungen schwierig zu rechtfertigen.

Entsprechend muss der Fachbeitrag aus wissenschaftlicher Sicht in seiner jetzigen Form als unvollständig zurückgewiesen werden.

Referenzen:

- [1] Schönwiese C.-D. „Analyse der Klimaänderungen in Hessen für den Zeitraum 1901–2003.“ 2012, in: INKLIM 2012 Baustein II – Klimawandel und Klimafolgen in Hessen, Abschlussbericht, Frankfurt/Main, 3–11.
- [2] Stocker, T.F.; et al. (eds.) „Climate Change 2013: The Physical Science Basis.“ Working Group 1 (WG1) Contribution to the Intergovernmental Panel on Climate Change (IPCC) 5th Assessment Report (AR5), 2014, Cambridge University Press.
- [3] Brasseur, G.P.; Jacob, D.; Schuck-Zöller, S. „Klimawandel in Deutschland: Entwicklung, Folgen, Risiken und Perspektiven“ 2017, Springer Spektrum.
- [4] Helmholtz Zentrum für Umweltforschung UFZ, Dürremonitor Deutschland, <https://www.ufz.de/>
- [5] Niederschrift über die 71. Verbandsversammlung, ZMW, 18.9.2012.

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