# FHI-aims Developers' and Users' Meeting 2026

ELECTRONIC STRUCTURE THEORY WITH NUMERIC ATOM-CENTERED BASIS FUNCTIONS

10.06.2026 – 12.06.2026

Max Planck Institute for the Structure and Dynamics of Matter (MPSD), Hamburg, Germany


Organizers:

Mariana Rossi, Volker Blum, Andrew Logsdail, Sebastian Kokott, Konstantin Mok Lion, Anna Lutz

MS1P
Molecular Simulations from First Principles e.V.

FHI-aims
The ab initio materials simulation package

# Information for Participants

## 1 Scope

This workshop will explore advanced methods in electronic structure development that are based on localized, numeric atom-centered orbitals (NAOs). NAO-based modeling is widely considered to be one of the most powerful approaches to studying molecules and materials from a first principles perspective. To advance the state of the art in this area, the proposed meeting will bring together key players from the FHI-aims code and related European and international efforts. Participants will have the opportunity to share their insights, discuss emerging trends, and collaborate on new research initiatives.

The workshop will cover three days and 24 invited talks, as well as a poster session. Time will be reserved in the afternoons for “Hands-On Discussions”, providing dedicated time for the participants to split up into small groups to focus on topics of specific interest ranging from methodological improvements all the way to code development questions related to specific subgroups of participants and joint programming sessions. Participants are also able to present their own work during the poster session.

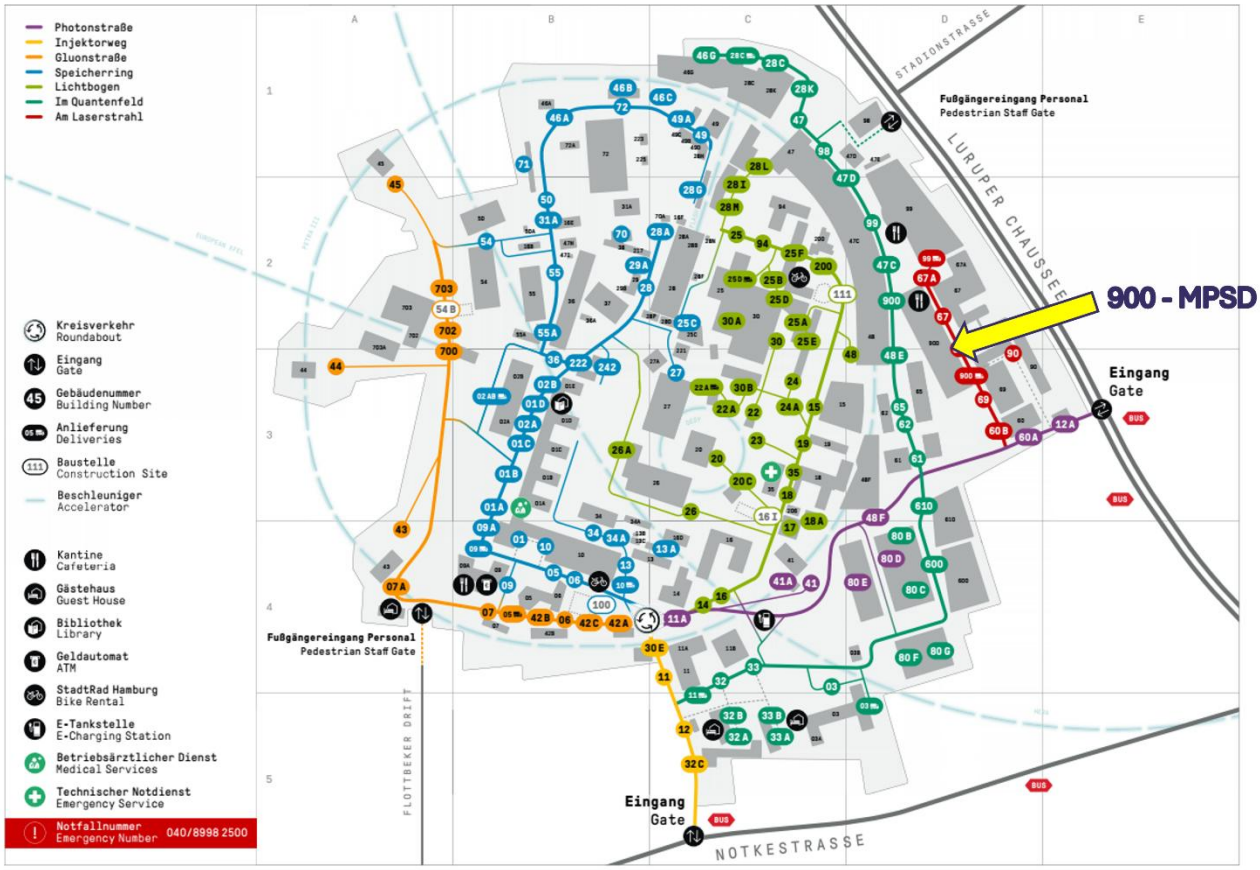
Topics covered are new developments in electronic structure theory with numeric atom-centered orbitals - including, but not limited to:

- Numerical algorithms and new methods for NAOs
- Technical advances in and scalability of electronic structure methods
- External libraries interfacing with FHI-aims
- Recent developments in advanced electronic properties

# 2 Conference Venue

The workshop will be held from June 10 – June 12, 2026 at

[Max Planck Institute for the Structure and Dynamics of Matter (MPSD)]
Rooms 131+136, Building 900
Luruper Chaussee 149, 22761 Hamburg



# 3 Program

| Wednesday, June 10, 2026 | |
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| 12:00 – 13:00 | Registration |
| 13:00 – 13:30 | **Volker Blum** (Duke University, USA) + **MS1P team**<br>*State of FHI-aims* |
| 13:30 – 13:55 | **Yosuke Kanai** (University of North Carolina at Chapel Hill, USA)<br>*New Developments with Nuclear-Electronic Orbital Method* |
| 13:55 – 14:20 | **Matthias Kick** (FHI, Germany)<br>*Large-Scale TDDFT for Finite and Periodic Systems* |
| 14:20 – 14:45 | **Hannah Bertschi** (MPSD, Germany)<br>*Ehrenfest Dynamics for Weakly-Bound Complexes in FHI-aims* |
| 14:45 – 15:15 | Coffee Break |
| 15:15 – 15:40 | **Ruiyi Zhou** (ETH Zurich, Switzerland)<br>*Recent Advances in Periodic BSE Calculations with Numeric Atom-Centered Orbitals* |
| 15:40 – 16:05 | **Contributed Talk 1: Jingkai Quan** (MPSD, Germany)<br>*Efficient band structure unfolding with atom-centered orbitals* |
| 16:05 – 16:30 | **Contributed Talk 2: Fabio Della Sala** (CNR-IMM, Italy) **Online**<br>*Adiabatic Connection Correlation Functionals from Hartree-Fock Orbitals* |
| 16:30 – 16:45 | Break |
| 16:45 – 18:15 | Hands-on Discussion 1 |
| 18:15 – 18:45 | Discussion Summary 1 |
| 18:45 – 19:00 | Break |
| 19:00 – 21:00 | Poster Session |

| Thursday, June 11, 2026 | |
|---|---|
| 09:00 – 09:25 | **Xinguo Ren** (Institute of Physics, CAS, China)<br>*RPA Correlation Energy at The Complete Basis Set Limit* |
| 09:25 – 09:50 | **Min-Ye Zhang** (Institute of Physics, CAS, China)<br>*All-electron low-scaling GW for periodic systems: interface, performance, and applications* |
| 09:50 – 10:15 | **Antonio Delesma** (University of Würzburg, Germany)<br>*A Low-Scaling RPA/GW Algorithm Based on Separable Resolution-of-the-Identity* |
| 10:15 – 10:45 | Coffee Break |
| 10:45 – 11:10 | **Moritz Leucke** (University of Würzburg, Germany)<br>*Resolution-of-the-Identity with Domain Decomposition* |
| 11:10 – 11:35 | **Danjo De Chavez** (University of Warwick, UK)<br>*Frozen Density Embedding Strategy in Numeric Orbital DFT* |
| 11:35 – 12:00 | **Gabriel A. Bramley** (Cardiff University, UK)<br>*Recent Advances in the EmbASI QM/QM Embedding Wrapper* |
| 12:00 – 13:30 | Lunch Break |
| 13:30 – 13:55 | **Noa Marom** (Carnegie Mellon University, USA)<br>*Structure Prediction of Organic/Inorganic Interfaces with Genarris* |
| 13:55 – 14:20 | **Subhayan Roychoudhury** (Avant-Garde Materials Simulation GmbH, Germany)<br>*Mastering organic crystal structure prediction for the infamous ROY molecule using the PBE0' hybrid functional* |
| 14:20 – 14:50 | Coffee Break |

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|---|---|
| 14:50 – 15:15 | **Christian Carbogno** (FHI, Germany)<br>*Beyond Ion Dynamics: Efficient Charge Transport Simulations including Electrons at Battery Scales* |
| 15:15 – 15:40 | **Elia Stocco** (MPSD, Germany)<br>*Scalable implementation of the Berry phase polarization with localized atomic orbitals* |
| 15:40 – 16:05 | **Wentao Zhang** (online, Duke University, USA)<br>*A Large-scale Parallel Implementation of Quasi-Four-Component Relativistic Density Functional Theory with Numeric Atom-centered Orbitals* |
| 16:05 – 16:15 | Break |
| 16:15 – 17:30 | Hands-on Discussion 2 |
| 17:30 – 18:00 | Discussion Summary 2 |
| 19:00 – 21:30 | Joint Dinner |

| **Friday, June 12, 2026** | |
|---|---|
| 09:00 – 09:25 | **Connor Box** (University of Cambridge, UK)<br>*Electron–Phonon Coupling and Superconductivity in FHI-aims* |
| 09:25 – 09:50 | **Krystof Brezina** (MPSD, Germany)<br>*Tip-Enhanced Raman Images of Realistic Systems Through Ab Initio Modeling* |
| 09:50 – 10:20 | Coffee Break |
| 10:20 – 10:45 | **María Camarasa-Gómez** (CFM Materials Physics Center, Spain)<br>*AI-Assisted Parameter Optimization in Density Functional Theory Calculations* |
| 10:45 – 11:10 | **Thomas Purcell** (University of Arizona, USA)<br>*Updates to the FHI-aims Python Environments* |
| 11:10 – 11:35 | **Tobias Henkes** (University of Luxembourg, Luxembourg)<br>*aims-PAX: Achieving Peace of Mind through Efficient & Automated Construction of Machine Learning Force Fields* |
| 11:35 – 12:00 | **Christoph Dähn** (FHI, Germany)<br>*Fantastic Polaronic Peaks and Where to Find Them: Learning Vibrational Spectra of a Disordered Energy Material* |
| 12:00 – 13:30 | Lunch Break |
| 13:30 – 13:55 | **Contributed Talk 3: Valdas Vitartas** (University of Warwick, UK)<br>*Uncertainty-Aware Machine Learning Hamiltonians with On-Demand SCF Refinement* |
| 13:55 – 14:20 | **Lydia Fichte** (FHI, Germany)<br>*DFT+U+V: Ground State and Real-Time Dynamics* |
| 14:20 – 14:45 | **Juhan Matthias Kahk** (University of Tartu, Estonia)<br>*Scalable Δ-Self-Consistent-Field Calculations of Core Electron Binding Energies in Periodic and Aperiodic Systems* |
| 14:45 – 15:30 | Coffee Break and Final Discussions |

# 4 Important Information

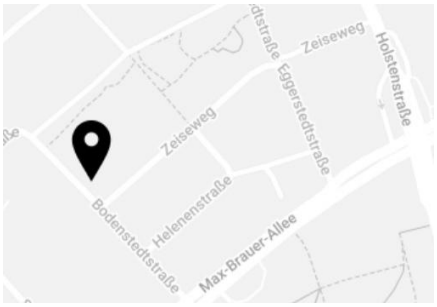
**Wi-Fi options at the MPSD site**

- **Eduroam**
- **„Science-Hotspot":** Open Wi-Fi network for guests on the DESY campus. No login credentials required.

**Conference Dinner**

The conference dinner will take place on Thursday, June 11, 19:00-21:30 at
Cantina fux&ganz
Bodenstedtstr 16
22765 Hamburg
https://fuxundganz.de/

The cantina can be reached in about 40 minutes by bus line M3 or X3 from "**Luruper Chaussee (DESY)**". Take either line M3 in direction "Kraftwerk Tiefstack" or line X3 in direction "U Meßberg" until "**S Holstenstraße**" and then walk for 10 minutes.
The main entrance of the cantina is at the corner Zeiseweg/ Bodenstedtstraße.



# 5 Talks

## 5.1 State of FHI-aims

**Opening and Invited Talk by Volker Blum and the MS1P team**

*Duke University, USA and MS1P e.V., Germany*

Welcome to the conference and an overview of where we are.

## 5.2 New Developments with Nuclear-Electronic Orbital Method

**Invited Talk by Yosuke Kanai**

*University of North Carolina at Chapel Hill, USA*

I will discuss some of our latest developments and applications of the nuclear-electronic orbital (NEO) method in Density Functional Theory (DFT), real-time time-dependent DFT (RT-TDDFT), and Bethe-Salpeter equation (BSE)/GW methods for investigating phenomena and systems in which proton quantum effects could be important.

## 5.3 Large-Scale TDDFT for Finite and Periodic Systems

**Invited Talk by Matthias Kick**

*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*

We present the implementation of linear-response Time-Dependent Density Functional Theory in the Tamm-Dancoff Approximation (TDA-TDDFT) within FHI-aims, supporting both finite and periodic systems. The implementation builds directly on FHI-aims' highly optimised hybrid DFT infrastructure, leveraging the localized resolution-of-identity approximation (RI-LVL) for the evaluation of exact exchange. This infrastructure, originally developed and benchmarked for ground-state hybrid functional calculations, has demonstrated substantial computational acceleration for large-scale non-periodic and periodic systems on massively parallel CPU clusters, and these capabilities are now extended into the time-dependent regime.
By inheriting and adapting these algorithmic advances, the present TDDFT implementation enables the efficient evaluation of excited state properties at the hybrid functional level for system sizes that were previously intractable within FHI-aims. This required modifications and extensions of the existing hybrid functional infrastructure to meet the specific demands of the time-dependent regime, including adaptations to the integral evaluation and screening strategies employed in the ground-state framework. Favorable computational scaling and a low memory footprint are achieved through the use of localized basis functions in combination with MPI3 shared memory arrays, which avoid redundant data replication across ranks within a node and enable efficient intra-node data sharing. Together, these design choices yield high parallel performance on modern HPC architectures.

We will discuss the key algorithmic aspects of the implementation, outline current capabilities for both molecular and periodic systems, and present benchmark results demonstrating accuracy and parallel efficiency. We further highlight the key differences and improvements relative to the existing TDDFT implementation in FHI-aims.

## 5.4 Ehrenfest Dynamics for Weakly Bound Complexes in FHI-aims

**Invited Talk by Hannah Bertschi**

*Max Planck Institute for the Structure and Dynamics of Matter, Germany*

Understanding how large-amplitude anharmonic nuclear motion influences electronic excitations is essential for explaining related phenomena in weakly bound systems. To model charge transfer and vibronic spectra in FHI-aims, we employ real-time time-dependent density functional theory [1] coupled to multitrajectory Ehrenfest dynamics. In this approach, nuclear anharmonicity is incorporated through the sampling of initial conditions. In contrast to more conventional methods, nuclear configurations and momenta are generated using quantum thermostat molecular dynamics with i-PI. This approach yields sampling of nuclear positions and momenta in close agreement with path-integral molecular dynamics at a cost comparable to classical molecular dynamics. We investigate the Mulliken and Hirshfeld charges of a water dimer on phenanthrene after excitation with an electric field. To describe the weak dispersion forces that hold this system together, we implemented the D3 [2] and TS [3] forces for Ehrenfest dynamics. We show that a 5 eV pulse leads, on average, to a transfer of electron density from phenanthrene to the water dimer. Moreover, we find that the nonadiabatic dynamics allows for a back-transfer of electron density to phenanthrene. [1] J. Hekele et al., J. Chem. Phys. 155, 154801 (2001) [2] S. Grimme et al., J. Chem. Phys. 132, 15410 (2010) [3] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett. 102, 073005 (2009)

## 5.5 Recent Advances in Periodic BSE Calculations with Numeric Atom-Centered Orbitals

**Invited Talk by Ruiyi Zhou**

*ETH Zurich, Switzerland*
*University of North Carolina at Chapel Hill, USA*

Many-body perturbation theory based on Green's functions has emerged as a powerful approach in both condensed matter physics and quantum chemistry. Within this framework, solving the Bethe-Salpeter equation (BSE) for the two-particle Green's function is the premier method for capturing particle-hole (exciton) interactions during electronic excitations. In standard BSE calculations, a static approximation to the screened Coulomb interaction kernel is typically employed. However, for systems with strong excitonic character—indicated by large exciton binding energies—dynamical screening effects become significant, rendering the static approximation inadequate. Solving the dynamical BSE for extended systems remains computationally prohibitive due to the dense Brillouin zone integration required.

In this talk, we present recent advancements in our newly developed all-electron implementation of the BSE@GW formalism for periodic extended systems, utilizing numeric atom-centered orbital (NAO) basis sets. [1, 2] Specifically, we formulate and implement an adaptation of the plane-wave-based effective dielectric function method [3] for dynamical BSE calculations within our NAO framework [4]. We validate this NAO-based dynamical BSE approach and demonstrate its realistic application by performing dynamical BSE@G0W0 calculations on the molecular crystal of naphthalene. Finally, we provide an outlook on future developments and applications of periodic BSE calculations using NAOs.

References

[1] Ruiyi Zhou*, Yi Yao*, Volker Blum, Xinguo Ren, and Yosuke Kanai. All-electron BSE@ GW method with numeric atom-centered orbitals for extended periodic systems. Journal of Chemical Theory and Computation, 21(1):291–306, 2024.

[2] Sampreeti Bhattacharya, Jianhang Xu, Ruiyi Zhou, and Yosuke Kanai. Proton quantum effects on electronic excitation in hydrogen-bonded organic solid: A first-principles green's function theory study. The Journal of Physical Chemistry Letters, 2026.

[3] Xiao Zhang, Joshua A Leveillee, and Andr´e Schleife. Effect of dynamical screening in the bethe-salpeter framework: Excitons in crystalline naphthalene. Physical Review B, 107(23):235205, 2023.

[4] Ruiyi Zhou*, Songrui Liu*, Jianhang Xu, Yao Yi, and Yosuke Kanai. All-electron Dynamical Bethe-Salpeter equation for extended systems with atom-centered orbital basis set. Submitted, 2026.

## 5.6 Efficient band structure unfolding with atom-centered orbitals

Jingkai Quan, Nikita Rybin, Matthias Scheffler, and Christian Carbogno

**Contributed talk by Jingkai Quan**

*Max Planck Institute for the Structure and Dynamics of Matter, Germany*

Band structure unfolding is a key technique for analyzing and simplifying the electronic band structure of large, internally distorted supercells that break the primitive cell's translational symmetry. In this work, we present an eficient band unfolding method for atomic orbital (AO) basis sets that explicitly accounts for both the nonorthogonality of atomic orbitals and their atom-centered nature. Unlike existing approaches that typically rely on a plane-wave representation of the (semi)valence states, we here derive analytical expressions that recast the primitive cell translational operator and the associated Bloch functions in the supercell AO basis. In turn, this enables the accurate and eficient unfolding of conduction, valence, and core states in all-electron codes, as demonstrated by our implementation in the all-electron ab initio simulation package FHI-AIMS, which employs numeric atom-centered orbitals. We explicitly demonstrate the capability of running large-scale unfolding calculations for systems with thousands of atoms and showcase the importance of this technique for computing temperature-dependent spectral functions in strongly anharmonic materials using CuI as example.

## 5.7 Adiabatic Connection Correlation Functionals from Hartree-Fock Orbitals

**Contributed Talk by Fabio Della Sala** **Online Talk**

*Institute for Microelectronics and Microsystems, CNR, Center for Biomolecular Nanotechnologies @UNILE, Italy*

The second-order Møller-Plesset correlation energy (MP2), which can be nowadays computed very efficiently, plays a central role in the development of the most accurate theoretical approaches for quantum chemistry and material science. Several double hybrid (DH) and adiabatic connection (AC) density functional methods, employing MP2 in the original or scaled/regularized/range-separated forms, have been proposed. However, in most of these approaches higher accuracy is obtained only with an empirical parameters, which are fitted to predefined benchmarks. Thus, the functional form can strongly depend on the type of systems and/or properties with more weight in the benchmarks, and, in addition, on the basis-set used for the calculations (which is critical for MP2).

Here, we construct correlation energy functional in the context of the Adiabatic Connection Integrand Interpolation (ACII) formalism, using only data from the strong-interaction regime, and thus without any empirical parameters from real systems. In constrast to DHs, ACII methods are non-linear functional of the MP2 correlation energy, thus allowing to treat also systems with vanishing-gap, and can be defined in term of Hartree-Fock or Exact-Exchange orbitals.

We present an accurate and throughout assessment at nearly complete basis-set limit, showing high accuracy of ACII functionals, for total correlation energy for small and large atoms, for surface energies, as well as for several quantum chemistry benchmarks.

We also show how to run ACII calculations in FHI-aims.

In addition, we present result for metallic bulk solids, from simple to transition metals. We show how to construct an ACII functional, which is correct for the uniform electron gas (UEG) as well as for the Wigner crystal limit, with an accuracy comparable to the best density-functionals, yet without any error cancellation on total energies.

References

L. A. Constantin, E. Fabiano, and F. Della Sala, Nonem- pirical adiabatic connection correlation functional from hartree–fock orbitals, The Journal of Physical Chemistry Letters 16, 3378 (2025).

Constantin, L. A.; Naeem, F.; Fabiano, E.; Sarcinella, F.; Della Sala, F. Restoring the point-and-charge gradient expansion for strong interaction density functionals. Phys. Rev. B (2026), 113, 085121,

F. Della Sala et al, submitted.

## 5.8 RPA Correlation Energy at The Complete Basis Set Limit

Hao Peng and Xinguo Ren

**Invited Talk by Xinguo Ren**

*Institute of Physics, Chinese Academy of Sciences, China*

Attaining reliable complete basis set (CBS) limit remains a significant challenge in ab initio correlated electronic-structure calculations. Building on our previous work for atoms and diatomic molecules, we present a finite-element (FE) Delta Sternheimer approach for numerically accurate random phase approximation (RPA) calculations applicable to general molecules. This approach seamlessly integrates atomic orbital basis sets with FE grids, enabling an arbitrarily precise representation of first order wavefunctions. As a result, the density response function and RPA correlation energies can be computed with fully controlled numerical precision. The Delta Sternheimer approach thus provides direct access to RPA correlation energies at the CBS limit, eliminating reliance on conventional extrapolation schemes. We apply this approach to two problems: The energy hierarchy of 20 water-dimer configurations and the atomization energies of 50 molecules from the G2 set, whereby incompleteness error of atomic orbital basis sets are rigorously assessed.

[1] H. Peng, S. Yang S, H. Jiang, H. Weng, and X. Ren, J. Chem. Theory Comput. 19, 7199 (2023).

[2] H. Peng and X. Ren, Phys. Rev. A. 112, 063819 (2025).

[3] H. Peng H, H. Liu, C. Li, H. Xie, and X. Ren, Phys. Rev. B, to be published; arXiv:2510.15570.

## 5.9 All-electron low-scaling GW method for periodic systems: Interface, performance, and applications

**Invited Talk by Min-Ye Zhang**

*Institute of Physics, Chinese Academy of Sciences, China*

The GW method is a powerful approach for predicting the electronic band structure of solids. However, its application to large-scale systems is often limited by the high computational cost. In FHI-aims, the conventional periodic GW implementation scales quartically with system size and does not exploit the matrix sparsity arising from the locality of numeric atom-centered orbitals (NAOs). In this talk, I present a low-scaling G^0W^0 implementation for periodic systems within the NAO framework, based on the space-time formalism and the local resolution-of-identity approximation. The method is implemented in LibRPA and interfaced with FHI-aims in an all-electron, full-potential framework. The talk introduces the underlying algorithm and outlines the design of LibRPA and its interface to FHI-aims. Benchmark results show the scaling behavior and parallel efficiency of the implementation relative to the canonical implementation in FHI-aims, with overall scaling close to O(N^{2.7}). Finally, the method is applied to the calculation of temperature-dependent spectral functions in strongly anharmonic systems.

## 5.10 A Low-Scaling RPA/GW Algorithm Based on Separable Resolution-of-the-Identity

**Invited Talk by Antonio Delesma**

*University of Würzburg, Germany*

We present an accurate low-scaling implementation of the random phase approximation (RPA) and $GW$. The method combines the space–time approach with a separable resolution-of-the-identity (RI) scheme [1] for the efficient evaluation of the irreducible polarizability. For the $GW$ self-energy, we employ the contour deformation technique together with analytic continuation of the screened Coulomb interaction ($W$), referred to as the CD–WAC method [2]. Benchmark calculations demonstrate excellent agreement with canonical reference implementations. For the Thiel test set, RPA total energies agree within 0.1 meV per electron. $GW$ quasiparticle energies for the GW100 test set show a mean absolute deviation of 1.1 meV. The present implementation reduces the computational scaling from $\mathcal{O}(N^{4})$ to $\mathcal{O}(N^{3})$ in practice. Combined with extensive GPU acceleration, this enables calculations for large atomic systems while retaining high accuracy. [1] J. Chem. Phys. 160, 024118 (2024). [2] J. Chem. Theory Comput. 19, 5450–5464 (2023).

## 5.11 Resolution-of-the-Identity with Domain Decomposition

**Invited Talk by Moritz Leucke**

*Universität Würzburg, Germany*

Four-center electron repulsion integrals appear in many electronic structure methods, such as many-body perturbation methods like the Random-Phase-Approximation or *GW* and others. To reduce their computational cost, the resolution-of-the-identity (RI) approximation is commonly employed. RI refactors the four-center integrals into three- and two-center integrals, among which the three-center integrals remain a computational bottleneck, particularly when using NAOs. We present a global RI scheme combined with a local metric (attenuated Coulomb) within an all-electron NAO framework, treating molecules and solids on equal footing. Central to the approach is a novel GPU-accelerated algorithm for computing 3-center integrals that relies on domain decomposition to improve load balancing and strong scaling. We demonstrate that our RI implementation achieves linear scaling with system size and maintains meV-level accuracy for *GW* energies. Performance benchmarks show scalability across thousands of CPU cores and substantial speedups with GPU support.

## 5.12 Frozen Density Embedding Strategy in Numeric Orbital DFT

**Invited Talk by Danjo De Chavez**

*University of Warwick, UK*

Multilevel embedding approaches provide a practical route to modeling extended materials by combining accurate quantum mechanical descriptions of chemically active regions with more economical treatments of their surrounding environments. In this work, we implement Frozen Density Embedding Theory (FDET) together with Freeze-and-Thaw (F&T) cycles in FHI-aims, enabling consistent embedding calculations for both cluster and periodic systems within the same framework. Initial subsystem densities are constructed from superpositions of free-atom densities. During the embedding procedure, one subsystem density is kept fixed while the other is variationally optimized, with iterative freeze–thaw cycles used to improve mutual polarization between subsystems. The implementation takes advantage of the efficient parallel infrastructure of FHI-aims. Both the embedding potential and subsystem densities are expanded using an auxiliary basis within a resolution-of-identity (RI) scheme, allowing efficient reconstruction on the real-space integration grid. The resulting framework enables the application of higher-level electronic structure methods to localized regions while retaining a density-functional description of the environment. This approach provides an efficient route to studying adsorption, bond dissociation, optical excitations, and charge-transfer processes relevant to surface catalysis and spectroscopy.

## 5.13 Recent Advances in the EmbASI QM/QM Embedding Wrapper

**Invited Talk by Gabriel Bramley**

*Cardiff University, UK*

Reducing the computational cost of electronic structure calculations while maintaining accuracy is a fundamental challenge for the computational chemistry community. Quantum mechanics in quantum mechanics (QM/QM) embedding methods address this concern by limiting the high-level calculation to a small region of chemical interest, while using less costly methods to represent the wider environment. This talk presents an open-source and modular Pythonic wrapper for implementing QM/QM embedding workflows in FHI-aims. The software, EmbASI, uses the ASI (Atomic Simulation Interface) API to efficiently communicate key data structures between FHI-aims and the wrapper. This communication protocol enables a general implementation of QM/QM embedding at the wrapper level with only minor code modifications to the FHI-aims codebase. We will demonstrate how QM/QM embedding techniques can effectively reduce the computational cost of post-Hartree-Fock treatments, including RPA and MP2, with minimal loss in accuracy. Furthermore, we will showcase recent developments in EmbASI, including support for spin-polarised and periodic systems.

## 5.14 Structure Prediction of Organic/Inorganic Interfaces with Genarris

**Invited Talk by Noa Marom**

*Carnegie Mellon University, USA*

Organic/inorganic interfaces perform critical functions in organic electronic devices and their structure can affect device performance. In addition, interactions with the substrate can promote the growth of otherwise metastable thin film structures by epitaxial templating. Predicting the structure of organic/inorganic interfaces by computer simulations can aid in the design of interfaces with desirable properties. We present Genarris Interfaces, a structure generator for organic/inorganic interfaces. Genarris uses epitaxy matrices to impose commensurism with the substrate. Film structures are generated in all layer groups that are compatible with the substrate symmetry and the requested number of molecules per unit cell. Clustering and down-selection are performed to reduce the number of structures while maintaining the diversity of packing motifs. Finally, relaxation and stability ranking are performed using dispersion-inclusive density functional theory (DFT). We demonstrate the application of Genarris for the interfaces of PTCDA on Ag(111), TCNE on Au(111), and naphthalene on Cu(111). In all cases, we find generated structures that resemble experimental scanning tunneling microscopy (STM) images. The electronic structure agrees well with spectroscopy experiments, where available. We envision Genarris Interfaces being used to predict the structure of organic/inorganic interfaces, to generate initial populations for other structure prediction algorithms, and to generate datasets for training machine learning models.

## 5.15 Mastering organic crystal structure prediction for the infamous ROY molecule using the PBE0' hybrid functional

**Invited Talk by Subhayan Roychoudhury**

*Avant-garde Materials Simulation Deutschland GmbH, Germany*

Ab initio prediction of the stability landscape of organic crystals has a massive importance for several real-world applications such as drug formulation. Here we will present a comprehensive overview of how, starting from a given organic molecule, DFT-based total-energy calculations using FHI-aims [1] are leveraged in a Crystal Structure Prediction (CSP) workflow designed by Avant-garde Materials Simulation (AMS), involving a cascade of energy-methods of varying degrees of complexity, that culminates in the generation of the temperature-dependent free energy landscape of crystals. As a case study, I will discuss the CSP for the highly polymorphic ROY molecule, for which several structures distort under semilocal functionals owing to the pronounced electron delocalization. I will discuss how an improved agreement with the experimental structures is obtained by energy minimizing with the PBE0' [2] functional in conjunction with a carefully parametrized dispersion correction within the Neumann-Perrin [3] formalism. I will also discuss how, with a combination of corrective energy methods and phonon calculations under strict convergence control, we produce the final TRHuST level free energy landscape [4] with the appropriate error bars. Finally, going beyond the thermodynamic regime, I will discuss the use of the state-of-the art crystallizability descriptor [5] to explore the kinetics of the crystallization of ROY.

I thank all members of the AMS team for their contributions to this project.

References
[1] V. Blum et al. “Ab initio molecular simulations with numeric atom-centered orbitals”. Comput. Phys. Commun. 180, 11 (2009), pp. 2175–2196. ISSN: 0010-4655.

DOI: https://doi.org/10.1016/j.cpc.2009.06.022.
1[2] S. Kokott, V. Blum, and M. Scheffler. “Efficient computation of the long-range exact exchange using an extended screening function”. The Journal of Chemical Physics 162, 22 (2025), p. 224103. ISSN: 0021-9606. DOI: 10.1063/5.0262451.

[3] M. A. Neumann and M.-A. Perrin. “Energy Ranking of Molecular Crystals Using Density Functional Theory Calculations and an Empirical van der Waals Correction”. J. Phys. Chem. B 109, 32 (2005), pp. 15531–15541. DOI: 10.1021/jp050121r.

[4] D. Firaha et al. “Predicting crystal form stability under real-world conditions”.
Nature 623 (2023), pp. 324–328. DOI: 10.1038/s41586-023-06587-3.

[5] J. van de Streek et al. “A conceptual framework for the crystallizability of organic compounds”.
J. Am. Chem. Soc. 147, 51 (2025). PMID: 41371992, pp. 46886–46896. DOI: 10.1021/jacs.5c08933.

## 5.16 Beyond Ion Dynamics: Efficient Charge Transport Simulations including Electrons at Battery Scales

**Invited Talk by Christian Carbogno**

*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*

Polarons, i.e., localized excess charges stabilized by lattice distortions, have long been recognized as fundamental to charge transport in energy materials. Nonetheless, a quantitative modeling of polaron dynamics has, so far, remained elusive in such materials. On the one hand, the activated dynamics of polarons requires time and length scales that are inaccessible to first-principles methods. On the other hand, off-the-shelf machine learned interatomic potentials (MLIPs) do not capture such electronic degrees of freedom. In this work, we overcome this hurdle proposing an MLIP model that explicitly accounts for these electronic degrees of freedom. The excess charge is incorporated into the MLIP as an independent degree of freedom that adiabatically follows the nuclear motion. We demonstrate the power of the approach for lithium titanium oxide (Li4Ti5O12 LTO), a prototypical anode material, for which polarons are known to play a key role [1]. We explore the PES for ionic diffusion in LTO using saddle-point search methods for different polaronic concentrations. By this means, we identify those barriers that are most affected by polarons. For these, we additionally perform accelerated free-energy calculations via umbrella sampling to shed light on the underlying mechanism that couples polaron and ion dynamics. This reveals that polarons in LTO do not merely serve as spectators, but lower the effective Li-diffusion barrier by thermodynamically adapting to the much slower ionic motion, resulting in an increase of conductivity by up to two orders of magnitude at room temperature. This is further substantiated by large-scale molecular-dynamics simulations, which also yield ionic and polaronic diffusion coefficients in line with experimental measurements. For the first time, this theoretically corroborates the occurrence of a correlated polaron-ion dynamics

with profound implications for the design of energy materials. [1] M. Kick, C. Scheurer, and H. Oberhofer, ACS Appl. Energy Mater. 4, 8583 (2021).

## 5.17 Scalable implementation of the Berry phase polarization with localized atomic orbitals

**Invited Talk by Elia Stocco**

*Max Planck Institute for the Structure and Dynamics of Matter, Germany*

Obtaining the polarization of materials from first-principles electronic structure calculations has become routine since the establishment of the modern theory of polarization. However, implementations based on the Berry-phase formalism are still largely concentrated in plane-wave electronic-structure codes, while implementations for atom-centered orbital frameworks remain comparatively rare.

This talk presents a scalable implementation of polarization calculations within the atom-centered numeric orbital framework of the FHI-aims code. Several aspects of the formalism that are specific to atom-centered basis sets are discussed, together with the algorithmic choices that enable efficient large-scale performance. In particular, the implementation achieves linear strong scaling with core count for systems containing more than 1000 atoms.

The presented approach extends efficient polarization calculations to large-scale simulations within atom-centered electronic-structure methods and enables applications to complex materials systems.

## 5.18 A Large-scale Parallel Implementation of Quasi-Four-Component Relativistic Density Functional Theory with Numeric Atom-centered Orbitals

**Invited Talk by Wentao Zhang** **Online Talk**

*Duke University, USA*

We present a large-scale parallel implementation of quasi-four-component (Q4C) relativistic densityfunctional theory with numeric atom-centered orbital basis sets for both molecules and periodic solids in the all-electron code FHI-aims. Our approach employs a domain decomposition method on nonuniform real space integration grids, which enables order-N integration of the Q4C Hamiltonian matrix elements using efficient, distributed-memory and compute-parallel real space operations. Next, we build the Hamiltonian and overlap matrices in a two-dimensional block-cyclic distribution layout. The resulting generalized eigenvalue problems are solved with the massively parallel ELPA eigenvalue solver library. We benchmark memory usage, parallel efficiency, and scalability across multiple MPI tasks and compute nodes. This algorithm extends the reach of fully relativistic DFT simulations for periodic solids well beyond 1,000 atoms per unit cell. As a demonstration, we calculate the fully relativistic band structure for a 1,504 atom-per-unit-cell doped hybrid organic-inorganic perovskite, (PEA)2(Pb1-xBix)I4 (PEA=phenethylammonium), showing the scalability and accuracy of this approach.

## 5.19 Electron–Phonon Coupling and Superconductivity in FHI-aims

**Invited Talk by Connor Box**

*University of Cambridge, UK*

Electron–phonon interactions play a central role in conventional superconductivity. Within Migdal–Eliashberg theory, the superconducting critical temperature T_c can be predicted from first principles using the electron–phonon spectral function, and this framework often provides reasonable agreement with experiment for conventional superconductors. Computational studies often focus on pristine materials with small primitive unit cells, where electron–phonon coupling is evaluated in reciprocal space using extremely dense q-point grids. While highly accurate, this approach becomes prohibitively expensive for realistic materials such as alloys, defects, or disordered systems that require large supercells. In this talk, I will present a real-space implementation of electron–phonon coupling and superconductivity within FHI-aims. Conceptually, the approach is not new: it builds on established Migdal–Eliashberg theory and finite-difference techniques that already exist within FHI-aims for phonons and electronic friction. However, by exploiting the localised, real-space basis of FHI-aims, the implementation naturally scales to large supercells and makes it possible to estimate superconducting properties for systems containing up to ~250 atoms. Our motivation is to move beyond idealised primitive-cell calculations and toward computational screening of more realistic materials. This opens the possibility of exploring superconductivity in complex environments such as alloys or chemically disordered systems that are difficult to treat with conventional reciprocal-space approaches. A central challenge is balancing accuracy and computational cost. In particular, adequately converging phonon properties in large supercells remains demanding. The goal of this work is therefore not necessarily maximal precision, but rather a practical framework capable of producing “good enough” estimates of T_cthat can be used to screen and identify promising conventional superconducting candidates

## 5.20 Tip-Enhanced Raman Images of Realistic Systems Through Ab Initio Modeling

**Invited Talk by Krystof Brezina**

*Max Planck Institute for the Structure and Dynamics of Matter, Germany*

Tip-enhanced Raman spectroscopy (TERS) is a powerful method for imaging vibrational motion and chemically characterizing surface-bound systems. Theoretical simulations of TERS images often consider systems in isolation, ignoring any substrate support, such as metallic surfaces. To enable efficient and accurate simulations of TERS on extended substrates, we developed a new, first-principles DFT-based methodology based on finite electric-field perturbations and implemented it in the FHI-aims software package. In this contribution, we discuss the theoretical foundations of our method and show that an ab initio description of the substrate and its interaction with molecular adsorbates is often critical. As examples of application, we use our method to predict TERS images of molybdenum disulfide monolayers in their pristine state and with sulfur vacancies and characterize the spectroscopic imprints of the defects. For Mg(II)-porphine on Ag(100), a system for which a direct

experimental comparison is possible, these simulations prove to be crucial for explaining the spatial variation of TERS intensity patterns and allow us to uncover fundamental principles of TERS spectroscopy. We explain how and why surface interactions affect images of out-of-plane vibrational modes much more strongly than those of in-plane modes, thereby providing an important tool for the future interpretation of these images in more complex systems.

## 5.21 AI-Assisted Parameter Optimization in Density Functional Theory Calculations

**Invited Talk by M. Camarasa-Gómez**

*CFM Materials Physics Center, Spain*

The accurate determination of optoelectronic properties of molecules and solids has been a central goal since the initial development of first-principles methods. This need has become even more pressing as the field of quantum materials rapidly advances, enabling breakthroughs in many different fields, such as energy-storage technologies, quantum devices, and biomedical sensing. A key challenge is the reliable prediction and characterization of electronic structure, where density functional theory (DFT) has long served as the standard computational tool. However, achieving the accuracy of many-body perturbation theory remains computationally demanding [1]. In this work, we explore a new strategy that couples modern artificial intelligence-driven optimization techniques with traditional DFT workflows [2]. By embedding these optimization methods directly into DFT workflows, we enable the automated adjustment of key functional parameters with the goal of improving both accuracy and efficiency. I will present our results obtained using various state-of-the-art optimization methods with surrogate models implemented in open-source libraries [3] and interfaced with FHI-aims, demonstrating their potential to accelerate and enhance first-principles electronic-structure predictions.

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[2] Á. Fraile-Carmona, D. Sánchez-Maqueda, C. Ramírez-Atencia, and M. Camarasa-Gómez (2025) [in preparation]
[3] J. Blank, and K. Deb, IEEE Access 8, 89497 (2020) *This work has been pursued in collaboration with Y. Aguirre-Ruiz, D. Sánchez-Maqueda, Á. Fraile-Carmona, and C. Ramírez-Atencia, from the Technical University of Madrid (Spain).

## 5.22 Updates to the FHI-aims Python Environments

**Invited Talk by Thomas Purcell**

*University of Arizona, USA*

Recent developments in the FHI-aims python environment and libraries have made significant changes to the backend, with minor updates for the user-facing environment. This talk will give a short overview of what the changes were made and how it will affect the FHI-aims community. Additionally , I will discuss new benchmarks for FHI-aims using some of the new changes. At the end

of the short introduction, I will lead a larger community discussion on the python environment and how the community wants to move forward.

## 5.23 aims-PAX: Achieving Peace of Mind through Efficient & Automated Construction of Machine Learning Force Fields

**Invited Talk by Tobias Henkes**

*University of Luxembourg, Luxembourg*

In recent years, machine learning force fields (MLFFs) have transformed molecular simulations. While pre-trained models are increasingly capable, there remains a strong demand for information-rich datasets to fine-tune general-purpose models or create custom ones for challenging applications. To this end, we introduce the ab initio molecular simulation Parallel Active eXploration (aims-PAX) package, an automated framework for constructing diverse and high-quality datasets for training MLFFs through active learning (AL). This software combines the electronic structure code FHI-aims with MLFFs, offering a user-friendly approach for efficient dataset creation. Through a parallelized, automated AL algorithm that leverages simultaneous sampling across multiple trajectories, our approach minimizes user intervention and optimizes computational resource use across CPU and GPU architectures. We demonstrate aims-PAX's capabilities across a range of challenging scenarios: autonomously identifying challenging systems within a defined chemical space; and enabling the simulation of solvated molecules comprising over 1,000 atoms by seamlessly handling both periodic and aperiodic systems. Lastly, we highlight the superior computational efficiency of the parallelized procedure on a perovskite system. The talk will also discuss how aims-PAX positions itself within the broader landscape of existing active learning and MLFF packages, highlighting its distinguishing design choices and advantages. Taken together, this work establishes aims-PAX as a powerful and versatile tool for advanced ML-driven atomistic simulations in both academic and industrial contexts, with the potential to grow alongside FHI-aims toward machine learning targets beyond force fields, such as electronic, optical, and other quantum mechanical properties.

## 5.24 Fantastic Polaronic Peaks and Where to Find Them: Learning Vibrational Spectra of a Disordered Energy Material

**Invited Talk by Christoph Dähn**

*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*

Vibrational Raman and infrared spectroscopy offers unique opportunities for characterizing microscopic structural and dynamical properties. For energy materials and in particular for solar batteries [1], a straightforward interpretation of such spectra is however hindered by the intrinsic structural and occupational disorder, which includes defects and polarons. At the same time, this also prevents their accurate ab initio simulation, which would require extensive calculations at a hybrid level of density-functional theory (DFT) in a multitude of disordered supercells. In this work, we discuss how machine-learning interatomic potentials trained on high-level DFT data can be used to

capture the otherwise inaccessible vibrational dynamics. We demonstrate this approach for a two-dimensional titanium niobate featuring partially occupied metal sites and polarons. By Monte Carlo sampling its configurational disorder, we are able to disentangle polaronic signatures and disorder induced contributions in the spectra. This reveals how local atomic environments control polaron stability and offers insights on how doping can be used to control charge retention in such compounds. [1] M. Rinaldi et al., J. Phys.: Mater. 8, 031003 (2025).

## 5.25 Uncertainty-Aware Machine Learning Hamiltonians with On-Demand SCF Refinement

**Valdas Vitartas**, Ben Saunders, Chen Qian, Lukas Hörmann, James R. Kermode, and Reinhard J. Maurer

**Contributed Talk by Valdas Vitartas**

*University of Warwick, UK*

The use of machine learning (ML) in computational sciences has grown in recent years, including machine learning interatomic potentials (MLIPs) that predict the energy as a function of geometry and composition of materials. However, the prediction of the energy alone is insuficient in application scenarios where an explicit description of the electronic structure is required, such as in electronic materials discovery. In this context, ML models have increasingly shifted towards predicting lower-level, solver-intrinsic quantities, such as the self-consistent Kohn-Sham Hamiltonian discretised in an atomic orbital basis [1]. On the other hand, extracting observables from an ML Hamiltonian requires additional, often expensive postprocessing, such as band structure calculations.
In this work, a workflow is presented that injects ML Hamiltonians back into FHI-aims via the Atomic Simulation Interface [2], enabling the use of optimised postprocessing routines such as ELSI-driven diagonalisation and band unfolding [3, 4]. Furthermore, the uncertainty of the Hamiltonian prediction is quantified and propagated to the eigenvalues, yielding uncertainty-aware quantities of interest. When the uncertainty exceeds a prescribed threshold, iterative self-consistent field (SCF) refinement is triggered within FHI-aims to control the risk associated with ML inference. The workflow is applied to investigate the configurational and compositional dependence on the electronic properties of nitrogen-doped graphene. Additionally, the analysis quantifies the calibration of predicted uncertainties and the time-to-solution gains compared to conventional density functional theory.

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## 5.26 DFT+U+V: Ground State and Real-Time Dynamics

**Invited Talk by Lydia Fichte**

*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*

Density functional theory (DFT) with a Hubbard correction (DFT+$U$ ) can mitigate self-interaction errors in a manner similar to hybrid functionals but at significantly lower computational cost. This makes extending DFT+$U$ to the time-dependent regime particularly attractive, as it allows for accurate simulations of electron dynamics at reduced computational expense. However, the on-site subspace defined by DFT+$U$ can be too rigid to describe phenomena involving strong orbital hybridization or charge transfer between sites, necessitating a more flexible definition of the correlated subspace. To address this, we are incorporating inter-site interactions through the +$V$ correction to enable a more complete and adaptable description. We are implementing an efficient real-time time-dependent DFT+$U$ +$V$ framework in FHI-aims, enabling accurate and scalable simulations of correlated electron dynamics. We discuss the current status of the implementation and highlight the pitfalls and intricacies encountered when working with a numeric atom-centered orbital basis, both in the ground state and in time-dependent simulations.

## 5.27 Scalable Δ-Self-Consistent-Field Calculations of Core Electron Binding Energies in Periodic and Aperiodic Systems

**Invited Talk by Juhan Matthias Kahk**

*University of Tartu, Estonia*

In a ΔSCF (Δ-Self-Consistent-Field) calculation, core electron binding energies are obtained as the difference between the total energies of the ground state, and the core hole final state. All-electron ΔSCF calculations of small molecules are well established. It has also been shown that the ΔSCF method can yield accurate core electron binding energies in more complex systems, like periodic solids and surface species. However, due to limitations of existing numerical implementations, such calculations are tedious for the user, and expensive to perform. In this talk, recent developments in the electronic structure code FHI-aims that integrate the routines for creating and tracking a localized core hole with the scalable Electronic Structure Infrastructure (ELSI) are presented. The new routines allow calculations of core-excited states with the same scalability as regular ground state DFT, enabling calculations of large systems, and the efficient use of parallel computing resources. In addition, periodic ΔSCF calculations now no longer require the use of wavefunction based restart files, which considerably simplifies the workflow for the user. Scalability tests of the new implementation, as well as applications to practical core electron binding energy calculations are presented.

# 6 Poster Abstracts

| Name | Affiliation | Poster Title |
|---|---|---|
| Esra Albar | Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany | Contour-Based Methods for Excited States of Large Systems |
| Jose Maria Castillo Robles | DTU Energy, Denmark | Modeling Lattice-Driven Li-Ion Migration in Garnet Electrolytes |
| Amit Chaudhari | Cardiff University, UK | A Multi-Task SISSO Approach for Automatic DFT+U Parameterisation in FHI-aims |
| Fredrik Eriksson | TU Wien, Austria | Defect-induced single-photon emitters in WSe2 |
| Peter Karpov | Max Planck Computing and Data Facility, Germany | Efficient distributed matrix multiplication on GPUs in ELPA |
| David Lara Vera | TU Dresden, Germany | Second-Variational Treatment of Spin-Orbit Coupling in GW Quasiparticle Calculations |
| Evgeny Moerman | University of Luxembourg, Luxembourg | Many-body contributions for accurate modeling of complex materials |
| Chris Shepard | University of North Carolina at Chapel Hill, USA | Hybrid XC functionals and other Developments in RT-TDDFT |
| Xuhao Wan | The NOMAD Laboratory at the FHI of the Max Planck Society, Germany | Physics-informed Neural Hamiltonians for Temperature-dependent Electrical Conductivity Calculations |
| Shuo Zhao | The NOMAD Laboratory at the FHI of the Max Planck Society, Germany | Building Trust in Ab Initio Machine-Learning Potentials for Extreme Materials – Applications to Strongly Anharmonic Ceramics and Thermal Insulators |

## 6.1 Contour-Based Methods for Excited States of Large Systems

**Esra Albar**

*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*

Traditional linear response methods use iterative techniques to compute each root one by one. In large and complex systems where the number of roots becomes very large this becomes computationally prohibitive. We propose using a contour-based subspace construction for the Rayleigh-Ritz procedure. These methods spans a limited set of eigenvalues rather than the full spectrum. This enables us to study the excited states of larger and more complex systems by extracting only peaks of interest. Our scheme entails further discussion of the symmetries of the target system and of how these symmetries may be exploited to guide the design of preconditioners, the selection of suitable eigensolvers, and the identification of the relevant spectral window.

## 6.2 Modeling Lattice-Driven Li-Ion Migration in Garnet Electrolytes

**Jose María Castillo Robles*,** Manuel Dillenz, Juan Maria García Lastra, Ivano E. Castelli

*Department of Energy Conversion and Storage, Technical University of Denmark*
*Anker Engelundsvej 411, DK-2800 Kgs. Lyngby, Denmark*
**Email:jmcro@dtu.dk*

Ion motion is central to the operation of lithium-ion batteries, dictating crucial performance metrics from charging rates to overall durability. However, the sluggish nature of macroscopic ion transport in solid-state electrolytes remains a critical bottleneck that fundamentally limits device performance. While empirical approaches, such as designing more polarizable lattices, have attempted to promote ion mobility, these strategies often face contradictory results and lack a unified theoretical foundation. Specifically, the role of lattice vibrations in facilitating ion transport remains one of the least experimentally explored areas, leaving a significant gap in our microscopic understanding. To address this, we combined ab initio molecular dynamics and nudged elastic band calculations to train a machine-learning interatomic potential for the prototypical garnet electrolyte LLZO. This computational approach enabled large-scale simulations with near-DFT accuracy, identifying specific vibrational modes that are strongly modulated during a Li-ion hop. Our molecular dynamics calculations revealed that ion migration is dynamically controlled by the instantaneous bottleneck geometry of the host lattice. To validate these computational insights, we directly compared our models against THz-pump and X-ray diffraction probe experiments. The experimental data confirmed our predictions, demonstrating that low-frequency THz radiation indirectly drives Li motion through optically active framework modes, while higher frequencies modify the time ions spend away from equilibrium positions. Furthermore, experiments pumping an IR-active mode established that framework motion remains phase-coherent for several cycles, corroborating our simulation finding that the migration bottleneck retains dynamical memory on transport-relevant timescales. Ultimately, this combined approach demonstrates how machine-learning-driven simulations, when rigorously validated by advanced experimental probes, can successfully unravel the complex

microscopic interplay between lattice dynamics and ion transport in next-generation battery materials.

## 6.3 A Multi-Task SISSO Approach for Automatic DFT+U Parameterisation in FHI-aims

**Amit Chaudhari[1],** Kushagra Agrawal, Akash Hiregange, Andrew J. Logsdail[2]

*Cardiff Catalysis Institute, School of Chemistry, Cardiff University, Cardiff, CF10 3AT, UK*
*[1]chaudharia@cardiff.ac.uk [2]logsdaila@cardiff.ac.uk*

Accurate defect simulations in transition metal oxides (TMOs) and rare-earth metal oxides (REOs) are crucial for the development of catalysts, batteries and solar cells for the energy transition. This requirement highlights a longstanding challenge in ab initio materials modelling, as semi-local density functional theory (DFT) often fails to capture the experimentally observed formation of defects and associated charge localisation (forming polarons) in these materials. In contrast, hybrid-DFT offers improved accuracy but is computationally intractable for large-scale simulations. Hubbard corrected DFT+*U* provides an efficient treatment for electron self-interaction errors in TMOs and REOs but relies on manually benchmarking multiple material-dependent parameters, including the Hubbard *U* value and projector, limiting its application across diverse materials.

To address this challenge, we present our work establishing a machine learning model for automatically determining Hubbard *U* values and projectors in open- and closed-shell TMOs and REOs within FHI-aims. Our approach uses multi-task symbolic regression and classification via the Sure Independence Screening and Sparsifying Operator (SISSO) algorithm [Ouyang et al., JPhys Mater., 2019] to learn a generalised mapping from bulk material structures to optimised Hubbard parameters, as defined by a latent representation of the hybrid-DFT electronic structure. The outcome is an analytical expression for the automatic parameterisation of material-dependent Hubbard *U* values and projectors that takes seconds to evaluate and is trained for broad generalisation across oxides of 18 transition metal and rare-earth elements. The work extends beyond our previous study in machine learning Hubbard projectors for accurate defect simulations in FHI-aims [Chaudhari et al., Digit. Discov., 2025] with the aim of establishing efficient reproducible workflows and pre-computed parameter defaults that are directly compatible with the existing DFT+*U* implementation [Kick et al., J. Chem. Theory Comput., 2019].

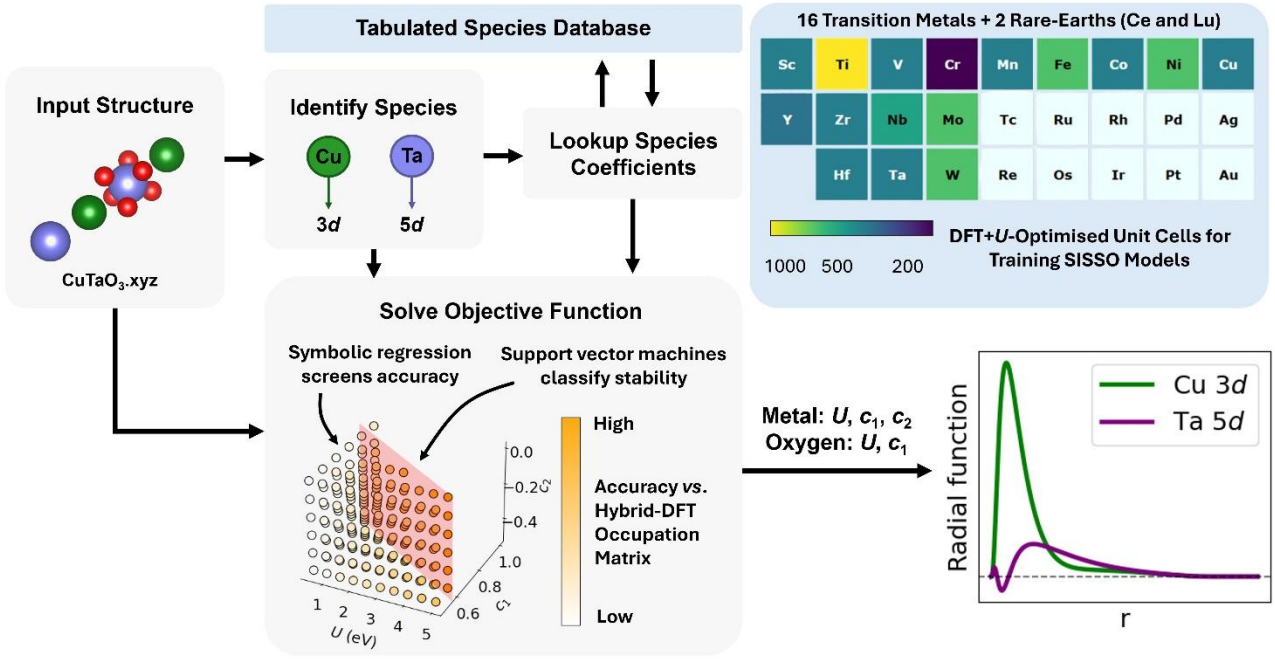


*Figure 1: Overview of automatic DFT+U parameterisation workflow from bulk material structures.*

## 6.4 Defect-induced single-photon emitters in WSe2

Sebastian Kindl[1], Max Sinner[2], Pablo Hernández López[3], **Fredrik Eriksson**[1], Sebastian Heeg[3], Florian Libisch[1]

*[1]TU Wien, [2]University of Luxembourg, [3]Humboldt-Universität zu Berlin*

Defects in two-dimensional semiconductors tune local optical properties, creating a promising platform for solid-state single-photon emitters. The complex interplay between electronic structure and lattice vibrations strongly influences optical stability, linewidths, and emission energies. Consequently, accurate modeling requires treatment of local defect states, localized defect phonons, and their interaction. Here, we consider electronic bandgap states of monolayer tungsten diselenide using a combined first-principles and machine-learning approach. Electronic structure calculations are performed with FHI-aims to accurately describe defect-induced in-gap states and their coupling to local structural distortions. To efficiently describe the localized electron-phonon interaction, we combine a MACE machine learned force field for energies and forces together with the MACE-H framework for localized Hamiltonians, both trained on first-principles data. We predict resulting signatures in photoluminescence measurements.

## 6.5 Efficient distributed matrix multiplication on GPUs in ELPA

**Peter Karpov,** Tobias Melson, Andreas Marek

*Max Planck Computing and Data Facility, Garching, Germany*

Distributed matrix-matrix multiplication is a fundamental building block of many dense linear algebra algorithms. While several multi-node, multi-GPU implementations exist, including SLATE [1], COSMA [2], and cuBLASMp [3], there is still lack of solution that is efficient, cross-platform, and optimized specifically for square matrices.

In ELPA [4] – a high-performance, MPI-parallel library with GPU acceleration for dense Hermitian eigenvalue problems – we have recently extended this functionality by introducing a GPU-capable distributed matrix multiplication based on the SUMMA algorithm [5]. The implementation utilizes an efficient "LCM-blocking" redistribution strategy [6] and GPU-aware communication paths, including NCCL and RCCL, in order to reduce communication overheads and improve performance in multi-GPU, multi-node environments.

As one application, we use the new matrix multiplication implementation to support mixed-precision iterative refinement for the computation of eigenvectors corresponding to non-degenerate eigenvalues, following the approach of Ogita and Aishima [7]. Our preliminary results indicate that, with the new distributed GPU multiplication available in ELPA, mixed-precision computations combined with iterative refinement can outperform native double-precision runs while still reaching double-precision accuracy.

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## 6.6 Second-Variational Treatment of Spin-Orbit Coupling in GW Quasiparticle Calculations

**David Lara Vera**

*Theoretical Chemistry, TU Dresden, Dresden, Germany*

Spin-orbit coupling (SOC) and many-body quasiparticle corrections are both essential for an accurate description of the electronic structure of materials with significant relativistic effects.
However, treating both effects simultaneously at full computational cost remains challenging. In this work, we present a post-processing scheme that applies second-variational SOC to GW quasiparticle energies within the FHI-aims framework. The approach builds on the standard second-variational SOC formalism, in which the SOC Hamiltonian is constructed in the basis of scalar-relativistic eigenstates. In our implementation, the diagonal part of the effective Hamiltonian is replaced by GW quasiparticle energies, while the SOC matrix elements are evaluated from the underlying scalar-relativistic wave functions. The resulting Hamiltonian is then diagonalized to obtain SOC-corrected quasiparticle states in an efficient and practical way. This strategy provides a computationally affordable route to combine GW accuracy with SOC-induced splittings, while avoiding the need for a fully relativistic GW treatment.

## 6.7 Many-body contributions for accurate modeling of complex materials

**Evgeny Moerman**, Ariadni Boziki, and Alexandre Tkatchenko

*University of Luxembourg, Luxembourg*

We present a systematic benchmark study of structural, mechanical, and electronic properties (lattice parameters, bulk moduli, adsorption distances, adsorption energies, and band gaps) for a diverse set of materials computed using combinations of density functional theory (DFT) exchange-correlation functionals (PBE and HSE06) and van der Waals (vdW) methods (D3, XDM, and MBD-NL). The computed properties are compared against experimental reference data to assess which level of theory is required for ab initio simulations to achieve quantitative agreement with experiment. Our results demonstrate that the hybrid functional HSE06 combined with the many-body dispersion (MBD-NL) method consistently yields the closest agreement with experiment across all tested systems and property classes. These findings underscore the importance of simultaneously incorporating a hybrid description of the electronic structure with an accurate many-body treatment of long-range van der Waals interactions. The generalized gradient approximation functional PBE, while computationally efficient, introduces systematic errors that are not fully remedied by pairwise vdW methods alone. Overall, our results establish MBD-NL as a robust and transferable framework for predictive materials modeling, providing clear guidance on the level of theory necessary for reliable first-principles calculations of complex materials.

## 6.8 Hybrid XC functionals and other Developments in RT-TDDFT

**Chris Shepard,** Jianhang Xu, Yosuke Kanai

*University of North Carolina at Chapel Hill, USA*

Over the past twenty years, real-time time-dependent density functional theory (RT-TDDFT) has emerged as an efficient first-principles method for studying electron dynamics in extended periodic systems[1]. Despite this progress, RT-TDDFT calculations still predominantly employ LDA and GGA exchange-correlation (XC) approximations, while ground-state DFT has increasingly adopted more sophisticated XC functionals, including hybrid XC functionals. Hybrid XC functionals, which incorporate some fraction of exact exchange, are known to improve key ground-state quantities as well as real-time observables such as the optical absorption spectrum. In this work we extend the localized resolution of identity (RI-LVL)[2] implementation of FHI-AIMS code in the context of RT-TDDFT, particularly for extended periodic systems. We first demonstrate that RI-LVL reproduces the results of the established RI-V method using isolated systems. We then discuss the implementation for extended periodic systems, contrasting with RT-TDDFT implementation in the Qb@ll/Qb@ch code based on plane-wave pseudopotential formalism. Finally, we detail other improvements in the RT-TDDFT section of the FHI-aims code.

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## 6.9 Physics-informed Neural Hamiltonians for Temperature-dependent Electrical Conductivity Calculations

**Xuhao Wan[a]*, Matthias Scheffler[a]***

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ABSTRACT
Predicting temperature-dependent electrical conductivity, σ(T), from first principles remains a major bottleneck for materials discovery: accurate transport calculations require either expensive electron–phonon workflows or dense quantum-mechanical response evaluations, and both scale poorly with structural complexity. We present a data-efficient, physics-informed workflow that enables accurate σ(T) prediction for crystalline materials by learning real space Hamiltonians from atomistic configurations and evaluating transport using the Kubo-Greenwood formalism.

Our approach couples molecular-dynamics sampling with an explicit data-quality strategy tailored to the sensitivity of Kubo-Greenwood transport. At representative temperatures, we generate configuration pools and apply stratified sampling using an anharmonicity metric σ to ensure coverage of rare but critical distortions. Across a representative set of SrTiO3 system, the resulting neural

Hamiltonians reproduce electronic structure features relevant to transport and deliver σ(T) in good agreement with experiment over broad temperature ranges, while reducing computational cost by orders of magnitude relative to conventional ab initio transport pipelines.

## 6.10 Building Trust in Ab Initio Machine-Learning Potentials for Extreme Materials – Applications to Strongly Anharmonic Ceramics and Thermal Insulators

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Thermal insulating ceramics and semiconductors often exhibit significant anharmonicity, particularly associated with rare events such as Frenkel defect creation and rattling phonon modes. These phenomena not only disrupt the phonon picture and the conventional perturbative methods for heat transport, but also pose challenges for the effective and trustful training of machine-learned interatomic potentials (MLIPs). Our contribution describes the implementation of a framework that combines the non-perturbative Green-Kubo formalism with a sequential, uncertainty guided active learning scheme using **AlmoMD**[1] with equivariant neural networks **NequIP**[2] and **So3krates**[3]. The approach is demonstrated by application to possibly ultra-low thermal conductivity materials[4]. Our results not only substantiate reliable predictions of thermal conductivity for strongly anharmonic systems but also pave the way for the accelerated exploration and design of
novel thermal insulators.

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