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## FHI-aims: Roadmap on Recent Advancements and Future Development Plans

Sebastian Kokott, James Green, Konstantin Lion, Andrei Sobolev, Yi Yao, Volker Blum<sup>b</sup>,  
Mariana Rossi<sup>a</sup>, Matthias Scheffler, and the world-wide FHI-aims community<sup>c</sup>

FHI-aims (Fritz Haber Institute ab initio materials simulations) [1,2,3] is a versatile electronic-structure software package developed for computational studies in molecular and materials science. Widely used by a global network of developers, researchers at the Fritz Haber Institute, academic institutions, and industry, FHI-aims leverages numeric atom-centered basis sets to deliver computational precision on par with leading benchmark codes for density functional theory (DFT) and many-body methods. Notably, it achieves this high level of precision [4] while retaining computational efficiency similar to plane-wave pseudopotential methods. The code demonstrates remarkable applicability, routinely handling systems comprising thousands of atoms with semi-local and hybrid density functionals – recently demonstrated up to 30.000 atoms for hybrid density functionals [5]. Additionally, it exhibits excellent scalability on modern high-performance computing platforms. FHI-aims boasts advanced electronic-structure capabilities for both molecules and solids and seamlessly integrates into complex simulation environments. This integration includes the ability to serve as a parallel library accessible through Python or via internet sockets or through its graphical user interface GIMS [6], making it a powerful tool for a wide range of scientific investigations. Recent updates include integration with high-throughput simulation frameworks like atomate2 (based on pymatgen) [7] and Taskblaster (based on ASE) [8], enhancing its capability to explore material properties efficiently. The FHI-aims community actively develops new features and interfaces with new external frameworks, such as dispersion correction models (XDM [9] and D3 [10]), band unfolding, the Kubo-Greenwood formula [11], crystal orbital overlap population analysis [12], and improvements to periodic GW calculations and to DFPT functionality, making FHI-aims a continuously evolving tool. As an outlook, we present a framework for active learning with SISSO [13], which is being tightly integrated with FHI-aims with the goal of broadening the usability of AI materials discovery.

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# Describing Complex Materials Properties and Functions via Materials Genes Identified by Artificial Intelligence

Lucas Foppa, Ray Miyazaki<sup>a</sup>, and Matthias Scheffler

A highly intricate interplay of underlying processes governs certain materials properties and functions. This prevents a realistic description by physical models or atomistic simulations. AI can identify nonlinear correlations between materials' parameters and the measured performance. Thus, AI might better capture the materials' behavior compared to the theory of the past. However, the data is often inconsistent and the flexibility of AI usually comes together with a lack of interpretability. To address these issues, we combine systematic experiments and simulations with interpretable, data-efficient AI to identify key physical parameters that describe complex materials properties, the "materials genes". [1] We discuss the concept and recent applications in heterogeneous catalysis. [2,3]

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# Sequential Active Learning Workflows for Materials Discovery Guided by Symbolic Regression: Identifying Acid-Stable Electrocatalysts

Akhil S. Nair, Lucas Foppa, and Matthias Scheffler

Sequential active learning (SAL)-driven workflows can efficiently guide experiments and simulations towards the discovery of materials with desired properties [1]. However, AI and machine-learning approaches commonly used in these workflows rely on the knowledge of key physical parameters describing the materials property of interest. These low-dimensional representations are typically unknown. Here, we address this challenge by developing a SAL workflow based on the sureindependence screening and sparsifying operator (SISSO) approach [2,3]. SISSO identifies, even based on moderate amounts of data, models for materials properties as analytical expressions depending on key parameters, out of many offered ones. Crucially, we train ensemble of SISSO models in order to obtain not only mean predictions, but also to quantify the uncertainty of the predictions, which are used to navigate the previously unexplored regions of materials space [4]. We demonstrate the SISSO-guided workflow by identifying acid-stable oxides for the water-splitting reaction by using high-quality DFT-HSE06 calculations [5].

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# Generality vs. Exceptionality: Optimal Sets of Subgroup Rules

## Describing CO<sub>2</sub> Activation on Single-Atom Alloys

Herzain I. Rivera-Arrieta, Lucas Foppa, Matthias Scheffler

Widely used machine-learning (ML) approaches in materials science and catalysis are designed to accurately describe, in average, a wide range of materials. Nonetheless, only a handful of compounds might show the desired properties to be suitable for a given application. Thus, global ML models may overlook these statistically exceptional materials of interest. Here, we discuss how the subgroup-discovery (SGD) approach can be utilized to identify descriptions focused on exceptional materials [1]. We present a systematic analysis of the Pareto front of optimal SGD solutions with respect to generality and exceptionality, two conflicting objectives in SGD [2]. The concepts are illustrated by the identification of “rules” describing single-atom alloys (SAAs) capable of providing a strong activation of adsorbed CO<sub>2</sub>, the first step towards the catalytic conversion of the molecule towards chemicals and fuels [3].

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# Electronic Band Structures at Finite Temperature with Unified Electron-Electron and Electron-Vibration Self-Energies

Min-Ye Zhang, Florian Merza<sup>a</sup>, Uthpala Herath<sup>b</sup>, Markus Rampp<sup>c</sup>, Volker Blumb, Xinguo Rend<sup>d</sup>, and Matthias Scheffler

An accurate first-principles description of the electronic band structure at finite temperatures is the prerequisite to quantitatively predict the electronic and optical properties of real materials. Theoretically, this requires proper consideration of the self-energy contributions from both electron-electron (e-e) and electron-vibration (e-vib) interactions. For the latter, the widely used electron-phonon coupling (EPC) model [1] fails for strongly anharmonic materials. Furthermore, while the self-energy contributions from the two types of interactions are considered separately within the EPC model, they can be treated collectively in a statistical manner [2] by combining the GW method with *ab initio* molecular dynamics. To realize this approach, a robust and efficient GW implementation for periodic systems is of key importance.

In this poster, we present our recent efforts to implement this approach to study electron self-energy using FHI-aims, an all-electron full-potential framework with compact numeric atom-centered orbitals (NAOs).[3] The one-shot periodic G0W0 method in FHI-aims is implemented based on the localized resolution-of-identity (RI) technique. [4,5] We first benchmark the performance of our G0W0 implementation in terms of accuracy and efficiency. We then show that a proper treatment of the dielectric response at long wave-length limit can significantly accelerate the convergence of quasiparticle band gap with respect to k-grids and auxiliary basis sets. Finally, using the band unfolding technique implemented in the NAO framework, we present temperature-dependent electronic band structure of silicon accounting for e-e and e-vib interactions, as a proof of concept.

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# Training Acceleration with Improved Reliability for Machine-Learned Interatomic Potentials via Active Learning Scheme: Strongly Anharmonic Thermal Insulator Examples

Kisung Kang, Shuo Zhao, Juan Zhang, Thomas A. R. Purcell<sup>a</sup>, Christian Carbogno, and Matthias Scheffler

Molecular dynamics (MD) has been popularly utilized to understand the dynamical properties of materials such as thermal, electrical, and ionic conductivities. Ab initio MD provides universal, high-quality predictions for energy, forces, and stress of any material, but its usage is limited due to high computational costs. Recent machine-learned interatomic potentials (MLIPs), with their excellent size scalability and remarkable calculation efficiency, can address this issue. However, the reliability of MLIPs could not be guaranteed for out-of-domain configurations. Particularly, rare events, such as defect creation or phase transition precursors, are often missed in training data or have regularized away due to insufficient data during MLIP training. But, owing to their significant impact on dynamical properties [1], their behavior should be reproduced by MLIP. This study systematically investigates how an active learning (AL) scheme can deal with rare event training and accelerate the whole training process [2]. First, the configurational space is examined by MD using explorative MLIPs, such as NequIP [3] and SO3KRATES [4]. Second, all generated MD snapshots are evaluated based on the MLIP prediction uncertainty, which enables qualitative identification of unfamiliar data. Finally, an iterative loop is formed by incorporating unfamiliar data into training data to retrain MLIP models for the next round. Applying AL to 122 materials [1, 5] identifies two representative corrections for erroneous MLIP predictions: a loss of real rare events and a prediction of false events. In addition, under-(over-) estimation of phonon lifetimes in AgGaSe<sub>2</sub>(CuI) shows the impact of erroneous MLIP predictions in dynamical properties, while AL rectifies them. In the end, we make NequIP enable the direct evaluation of unfolded heat flux prediction via automatic differentiation [6], resulting in efficient heat conductivity evaluation using MLIPs. Finally, a whole AL process leads to a systematic MLIP approach for thermal conductivity predictions of thermal insulators.

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# Non-perturbative Electronic Transport for Strongly Anharmonic Materials

Jingkai Quan<sup>a</sup>, Christian Carbogno, and Matthias Scheffler

First-principles approaches for phonon-limited electronic transport are typically based on many-body perturbation theory [1] and thus rely on the validity of a quasi-particle picture for phonons and electrons. However, both these pictures can become questionable in strongly anharmonic systems [2,3]. We overcome this hurdle by combining *ab initio* molecular dynamics (aiMD) calculations with the Kubo-Greenwood (KG) formalism [4]. This non-perturbative, stochastic method allows us to account for all orders of anharmonic and vibronic couplings in the calculation of carrier mobilities. We discuss the implementation of this formalism in the *ab initio* material simulation package FHI-aims [5] and the strategy to extrapolate to the direct current limit [6]. Furthermore, to analyze the impact of strong electron-nuclei interactions on the electronic structure, we also developed an efficient band unfolding method for linear combination of atomic-centered orbital (LCAO) basis sets [7], enabling us to define a non-perturbative, temperature-dependent electronic spectral function. Finally, we demonstrate the capabilities of these methods by calculating and analyzing the temperature-dependent electron mobility of the strongly anharmonic oxide perovskites SrTiO<sub>3</sub> and BaTiO<sub>3</sub> across a wide range of temperatures [8].

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