Code Developments

FHI-aims 250822 Release

- A new FHI-aims release, 250822, is now available for download on aimsclub. This release incorporates numerous new features (including Superconductivity module by Connor Box, and implementation of relativistic Q4C with Scalapack by Wentao Zhang, amongst others) and important bug fixes, made possible through the valued contributions of our community. For a comprehensive overview of all changes, please refer to the CHANGELOG

Wentao Zhang

- Implementation of relativistic q4c with use_scalapack + use_local_index, reducing the memory usage for large periodic systems.
- New exact four component density matrix based density update method for both large and small components density in q4c for all current implemented FHI-aims matrix storage formats. A new keyword, q4c_small_dens_update is added (default value is .true.). This controls whether to use the new update method or not (corresponding to previous q4c code). The default is to use new method. (**breaking change**)
- Band structure can be calculated at q4c level of theory for systems of up to 1500 atoms. MR !1942

Connor Box

- Refactored friction module to reduce memory usage significantly. Some changes to the superconductivity module. MR !1929
- Various bugfixes for friction module MR !1935, MR !1937, MR !1941, MR !1943, MR !1951

Konstantin Lion

- Bugfix for slab identification with translated unit cells during a geometry relaxation MR !1922

Muhammad Tahir

- Improvements to RPA forces MR !1925, MR !1926, MR !1927, MR !1930, MR !1934, MR !1940MR !1944, MR !1945

Jakob Filser

- Environ improvements MR !1931, MR !1933

James Green

- Bugfix for elsi_restart_use_overlap with the LAPACK code branch MR !1932

Hannah Bertschi

- Add D3 dispersion corrections to Ehrenfest dynamics MR !1952

Jonas Brandhoff

- Implementation of Mayer bond order calculation via an external script, described in Section 3.45.3 of the FHI-aims manual MR !1939

Thomas Purcell

- Add missing # in the Mn species defaults to not break pyfhiaims MR !1947

New Software Involving FHI-aims

aims-PAX

- aims-PAX, short for ab initio molecular simulation-Parallel Active eXploration, is a flexible, fully automated, open-source software package for performing active learning for machine learning force fields using a parallelized algorithm that enables efficient resource management.

- It is described in the following pre-print available on arXiv: "aims-PAX: Parallel Active eXploration for the automated construction of Machine Learning Force Fields" by Tobias Henkes, Shubham Sharma, Alexandre Tkatchenko, Mariana Rossi, and Igor Poltavskyi, https://arxiv.org/abs/2508.12

MACE4IR

- MACE4IR is a foundational model, capable of rapid and reliable prediction of IR spectra.
- It is trained on 10 million geometries and corresponding FHI-aims DFT energies, forces and dipoles from the Google DeepMind QCML database, and validated against further FHI-aims DFT calculations. It can predict IR spectra for organic, inorganic, metal complexes and biologically relevant species at a fraction of the cost of DFT calculations.
- It is described in the following pre-print available on arXiv: "MACE4IR: A foundation model for molecular infrared spectroscopy", by Nitik Bhatia, Ondrej Krejci, Silvana Botti, Patrick Rinke, and Miguel A. L. Marques, https://arxiv.org/abs/2508.19118

New Papers involving FHI-aims

Disclaimer: We compile this list by identifying recent publications that cite the 2009 FHI-aims paper (DOI: 10.1016/j.cpc.2009.06.022). Before including any publication, we verify that FHI-aims was used in some capacity within the article. If we have overlooked any published work involving FHI-aims, we apologize for the oversight and welcome you to inform us. This list is intended for informational purposes only.

- "Out-of-Plane Rashba Spin-Splitting and Structure-Property Relationships in Layered Cu2AMVSe4 Chalcogenides (A = K, Rb, Cs; MV = V, Nb, Ta)", Timothy M. McWhorter, Wentao Zhang, Yang Shen, Volker Blum, and David B. Mitzi, Chemistry of Materials, (2025) in press, DOI: 10.1021/acs.chemmater.5c01116

- "Taskblaster: a generic framework for automated computational workflows", Ask Hjorth Larsen, Mikael J. Kuisma, Tara M. Boland, Fredrik A. Nilsson and Kristian S. Thygesen, Digital Discovery, (2025) in press, DOI: 10.1039/D5DD00097A

- "Constrained nuclear–electronic orbital method for periodic density functional theory: Application to H2 chemisorption on Si(001) surfaces", Songrui Liu, Jianhang Xu, and Yosuke Kanai, J. Chem. Phys. 163, 084110 (2025), DOI: 10.1063/5.0278375

- "Predicting dynamic spin splitting in 2D hybrid organic-inorganic perovskites via machine learning model", Sampreeti Bhattacharya, Aidan J. Thomas, and Yosuke Kanai, Chem. Phys. Rev. 6, 031402 (2025), DOI: 10.1063/5.0261959

- "Tuning Conductance in BODIPY-Based Single-Molecule Junctions", Emma York, Ilana Stone, Wanzhuo Shi, Xavier Roy, and Latha Venkataraman, Nano Letters, (2025), in press DOI: 10.1021/acs.nanolett.5c03764

- "Origins of electrical conductivity in 3D iron-tetrazole-based metal–organic frameworks", María Esteve-Rochina, Jennifer Faro-Guara, Enrique Ortí, Aron Walsh, and Joaquín Calbo, J. Mater. Chem. C, (2025), in press, DOI: 10.1039/D5TC02135A

- "Mechanochemical Alloying of Molecular Dopants in Expanded Analogs of Halide Perovskites", Xavier Rodriguez-Rubio, Giovanni Vescio, Joshua D. Forero, Albert Cirera, Horst Puschmann, Eliseo Ruiz, Sergi Hernández, and Roc Matheu, Inorganic Chemistry, 64, 17279-17287, (2025), DOI: 10.1021/acs.inorgchem.5c02436

- "Interaction strength of carbon dioxide on graphene from periodic quantum diffusion Monte Carlo", Flaviano Della Pia, Giaan Kler-Young, Andrea Zen, Fabian Berger, Dario Alfè, Angelos Michaelides, J. Chem. Phys., 163, 071101, (2025), DOI: 10.1063/5.0283254

- "Controlled Incorporation of Silver Atoms into Coordination Chain Single-Molecule Junctions Formed on Gold Electrodes", Zelin Miao and Maria Kamenetska, Nano Letters, 25, 12979-12986, (2025), DOI: 10.1021/acs.nanolett.5c03157

- "Chiral Phonon-Induced Spin Transport via Microscopic Barnett Effect", Xixi Qin, Cong Yang, Dali Sun, Jun Liu, and Volker Blum, Phys. Rev. Lett. 135, 076703, (2025), DOI: 10.1103/kp6b-2kxz

- "The mechanisms of preferential occupation and planar defect transformation in the mu phase of cobalt-based superalloys", Wei Chen, Yunsong Zhao, Xiaoyu Fei, Xiuyuan Wang, Pengfei Nan, Yongsheng Zhang, Huixin Jin, and Binghui Ge, 298, 121399, (2025), DOI: 10.1016/j.actamat.2025.121399

Upcoming Events

- Save the date: New webinar on September 03 and 04 on "Explainable AI models for Materials Science with the SISSO Approach" with talks by Tom Purcell and Lucas Foppa

- Next FHI-aims monthly meeting: WEDNESDAY Oct 01, 2025 0930 AM Eastern Time, US and Canada, more details in the community Slack channel