

FHI-aims Developers' & Users' Meeting 2026

JUNE 10 – 12, 2026 · PROGRAM

Wednesday June 10, 2026

12:00–13:00 REGISTRATION

13:00–13:30 Volker Blum + MS1P team **OPENING**

Duke University, USA + MS1P e.V., Germany

State of FHI-aims

13:30–13:55 Yosuke Kanai

UNC Chapel Hill, USA

Nuclear-Electronic Orbital Method

13:55–14:20 Matthias Kick

FHI, Germany

Large-Scale TDDFT for Finite and Periodic Systems

14:20–14:45 Hannah Bertschi

MPSD, Germany

Ehrenfest Dynamics for Weakly-Bound Complexes

14:45–15:15 COFFEE BREAK

15:15–15:40 Ruiyi Zhou

ETH Zurich, Switzerland

Periodic BSE with Numeric Atom-Centered Orbitals

15:40–16:05 Jingkai Quan **CONTRIBUTED TALK**

MPSD, Germany

Efficient band structure unfolding with atom-centered orbitals

16:05–16:30 Fabio Della Sala **CONTRIBUTED TALK** **ONLINE**

CNR-IMM, Italy

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

RPA Correlation Energy at The Complete Basis Set Limit

09:25–09:50 Min-Ye Zhang

Institute of Physics, CAS, China

All-electron low-scaling GW for periodic systems

09:50–10:15 Antonio Delesma

University of Würzburg, Germany

Low-Scaling RPA/GW Based on Separable RI

10:15–10:45 COFFEE BREAK

10:45–11:10 Moritz Leucke

University of Würzburg, Germany

Resolution-of-the-Identity with Domain Decomposition

11:10–11:35 Danjo De Chavez

University of Warwick, UK

Frozen Density Embedding in Numeric Orbital DFT

11:35–12:00 Gabriel A. Bramley

Cardiff University, UK

Advances in the EmbASI QM/QM Embedding Wrapper

12:00–13:30 LUNCH BREAK

13:30–13:55 Noa Marom

Carnegie Mellon University, USA

Structure Prediction of Organic/Inorganic Interfaces

13:55–14:20 Subhayan Roychoudhury

Avant-Garde Materials Simulation, Germany

Crystal structure prediction for ROY using PBE0'

14:20–14:50 COFFEE BREAK

14:50–15:15 Christian Carbogno

FHI, Germany

Charge Transport incl. Electrons at Battery Scales

15:15–15:40 Elia Stocco

MPSD, Germany

Scalable Berry phase polarization

15:40–16:05 Wentao Zhang **ONLINE**

Duke University, USA

Q4C Relativistic DFT 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

Electron-Phonon Coupling and Superconductivity

09:25–09:50 Krystof Brezina

MPSD, Germany

Tip-Enhanced Raman via Ab Initio Modeling

09:50–10:20 COFFEE BREAK

10:20–10:45 María Camarasa-Gómez

CFM Materials Physics Center, Spain

AI-Assisted Parameter Optimization in DFT Calculations

10:45–11:10 Thomas Purcell

University of Arizona, USA

Updates to the FHI-aims Python Environments

11:10–11:35 Tobias Henkes

University of Luxembourg

aims-PAX: Efficient & Automated Construction of ML Force Fields

11:35–12:00 Christoph Dähn

FHI, Germany

Fantastic Polaronic Peaks: Learning Vibrational Spectra of a Disordered Energy Material

12:00–13:30 LUNCH BREAK

13:30–13:55 Valdas Vitartas **CONTRIBUTED TALK**

University of Warwick, UK

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

13:55–14:20 Lydia Fichte

FHI, Germany

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

14:20–14:45 Juhan Matthias Kahl

University of Tartu, Estonia

Scalable Δ SCF Core Electron Binding Energies

14:45–15:30 COFFEE & FINAL DISCUSSIONS