FHI-aims Developers' & Users' Meeting 2026

JUNE 10 – 12, 2026 · PROGRAM

Wednesday June 10, 2026

12:30–13:00 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

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
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
Complete basis set limit in all-electron RPA and GW

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 Kahk
University of Tartu, Estonia
Scalable ΔSCF Core Electron Binding Energies

14:45–15:30 COFFEE & FINAL DISCUSSIONS