

MMBI15 WORKSHOP SCIENTIFIC PROGRAM

Tuesday Afternoon (May 26, 2:00 PM – 6:00 PM)

2:00 PM – 2:30 PM

Alexandre Tkatchenko

Fritz-Haber-Institut der Max-Planck-Gesellschaft (Germany)

Opening Remarks & Logistics

2:30 PM – 3:10 PM

Christian Wagner

Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich (Germany)

Probing van der Waals Potentials with Controlled Molecular Manipulation

3:10 PM – 3:50 PM

Alberto Ambrosetti

University of Padova (Italy)

Wavelike Nature of van der Waals Interactions at the Nanoscale

3:50 PM – 4:15 PM

Coffee Break

4:15 PM – 4:55 PM

Anthony Reilly

Cambridge Crystallographic Data Centre (UK)

Many-Body van der Waals Interactions in Molecular Materials: Stabilities, Polymorphism, and Beyond

4:55 PM – 5:20 PM

Jan Hermann

Fritz-Haber-Institut der Max-Planck-Gesellschaft (Germany)

Many-Body Dispersion Meets Non-Local Density Functionals: Towards a Unified Approach for van der Waals Correlations

5:20 PM – 6:00 PM

Sameer Varma

University of Southern Florida (USA)

Many-Body Effects in Biomolecular Ionic Interactions

MMBI15 WORKSHOP SCIENTIFIC PROGRAM

Tuesday Evening (May 26, 8:00 PM – 10:00 PM)

8:00 PM – 10:00 PM

Poster Session

- Mikhail Askerka, *Yale University (USA)*
Electron-Hole Pair Coupling Induced Vibrational Relaxation of Molecules on Metal Surfaces
- Mausumi Chattopadhyaya, *Fritz-Haber-Institut der Max-Planck-Gesellschaft (Germany)*
How Molecules Interact Through Nanostructures
- Nicola Ferri, *Fritz-Haber-Institut der Max-Planck-Gesellschaft (Germany)*
Electronic Properties of Materials with a Self-Consistent Interatomic van der Waals Density Functional
- Vivekanand Gobre, *Fritz-Haber-Institut der Max-Planck-Gesellschaft (Germany)*
Many-Body Electrodynamical Response for Molecules and Materials from the Ground-State Electron Density
- Johannes Hoja, *Fritz-Haber-Institut der Max-Planck-Gesellschaft (Germany)*
Phonons in Molecular Crystals and Their Coupling to Collective Electronic Fluctuations
- Fairaja Kabeer, *Fritz-Haber-Institut der Max-Planck-Gesellschaft (Germany)*
Role of van der Waals Interactions in Catalytic Processes at Surfaces
- Hsin-Yu Ko, *Princeton University (USA)*
Anharmonic Effects from Dispersion in Weakly Bound Molecular Crystals
- Xiaofei Liu, *Fritz-Haber-Institut der Max-Planck-Gesellschaft (Germany)*
Elucidating Negative Linear and Area Compressibility in Metal-Organic Frameworks
- Victor Lopez, *Fritz-Haber-Institut der Max-Planck-Gesellschaft (Germany)*
Density-Functional Theory with Screened van der Waals Interactions for the Modeling of Hybrid Inorganic/Organic Systems
- Gionni Marchetti, *Fritz-Haber-Institut der Max-Planck-Gesellschaft (Germany)*
Machine Learning and Quantum Mechanics
- Limin Zheng, *Fritz-Haber-Institut der Max-Planck-Gesellschaft (Germany)*
Theoretical Studies of the Intermolecular Interaction in the OCS-CO₂ Complex

MMBI15 WORKSHOP SCIENTIFIC PROGRAM

Wednesday Morning (May 27, 9:30 AM – 12:30 PM)

9:30 AM – 10:10 AM

Pier Luigi Silvestrelli

University of Padova (Italy)

Adsorption on Transition Metals by van der Waals Corrected DFT: Xe and Graphene on Ni(111)

10:10 AM – 10:50 AM

John Parkhill

University of Notre Dame (USA)

Non-equilibrium Realtime TD-DFT and Application to Lead-Halide Perovskites

10:50 AM – 11:25 AM

Coffee Break

11:25 AM – 12:05 PM

Ignacio Franco

University of Rochester (USA)

Electronic Decoherence in Molecules

12:05 PM – 12:30 PM

Bartomeu Monserrat

Cambridge University (UK)

Searching for Saddle Points: Vibrationally Stabilised Structures

MMBI15 WORKSHOP SCIENTIFIC PROGRAM

Wednesday Afternoon (May 27, 2:00 PM – 5:00 PM)

2:00 PM – 5:00 PM

Free Time

MMBI15 WORKSHOP SCIENTIFIC PROGRAM

Thursday Morning (May 28, 9:30 AM – 12:30 PM)

9:30 AM – 10:10 AM

Volker Blum

Duke University (USA)

Quantitative at Last? Accurate All-Electron Dispersion Corrected DFT “Gets” Complex Molecules and Functional 2D Materials

10:10 AM – 10:35 AM

Martin Blood-Forsythe

Harvard University (USA)

Analytical Nuclear Gradients for the Range-Separated Many-Body Dispersion Model of Non-covalent Interactions

10:35 AM – 11:00 AM

Thomas Markovich

Harvard University (USA)

Enabling Large-Scale Simulation of Many-Body Dispersion Forces in Condensed-Phase Systems

11:00 AM – 11:25 AM

Coffee Break

11:25 AM – 11:50 AM

Biswajit Santra

Princeton University (USA)

Predicting Anomalous Properties of Water Using *Ab Initio* Molecular Dynamics

11:50 AM – 12:30 PM

Ryan Steele

University of Utah (USA)

Exploiting the Timescales of Molecular Interactions for Enhanced *Ab Initio* Molecular Dynamics

MMBI15 WORKSHOP SCIENTIFIC PROGRAM

Thursday Afternoon (May 28, 2:00 PM – 5:30 PM)

2:00 PM – 2:40 PM

Gregory Beran

University of California, Riverside (USA)

The Challenges of Modeling Three-Body Intermolecular Interactions

2:40 PM – 3:20 PM

Yihan Shao

National Institutes of Health (USA)

Decomposition of Molecular Polarizability and Estimation of QM/MM Polarization Energy

3:20 PM – 4:00 PM

Coffee Break

4:00 PM – 4:25 PM

Tristan Bereau

Max Planck Institute for Polymer Research (Germany)

To Hell with Parametrization: Toward Physics-Based and Data-Driven Classical Force Fields

4:25 PM – 4:50 PM

Andrew Simmonett

National Institutes of Health (USA)

Efficient Treatment of Multipoles and Induced Dipoles

4:50 PM – 5:30 PM

Glenn Martyna

IBM Thomas J. Watson Research Center (USA)

The Quantum Drude Oscillator Model for Linear Scale Atomistic Simulation—A Coarse Grained Electronic Structure Allowing for High Environmental Transferability

MMBI15 WORKSHOP SCIENTIFIC PROGRAM

Friday Morning (May 29, 9:30 AM – 12:00 PM)

9:30 AM – 10:10 AM

Francesco Paesani

University of California, San Diego (USA)

Many-Body Approaches to Vibrational Spectroscopy

10:10 AM – 10:35 AM

Reinhard Maurer

Yale University (USA)

Many-Body Interactions in Dynamics of Molecules on Surfaces

10:35 AM – 11:05 AM

Coffee Break

11:05 AM – 11:30 AM

Igor Poltavskyi

Fritz-Haber-Institut der Max-Planck-Gesellschaft (Germany)

Converged Nuclear Quantum Statistics from Semiclassical Path Integral Molecular Dynamics

11:30 AM – 12:00 PM

Robert A. DiStasio Jr.

Princeton University (USA)

Closing Remarks & Logistics