

Day 1 **14-Oct**

8:50 9:00 Welcome

The complexity of molecules on surfaces

9:00 9:40 Stefan Tautz Precise adsorption energies and molecule-surface van der Waals potentials from force measurements

9:40 10:20 Nikolaj Moll Imaging Atoms and Bonds by Atomic Force Microscopy

Break

10:50 11:30 Michael Rohlfing Structure and spectra of organic molecules on silver from first principles

11:30 12:10 Leeor Kronik The derivative discontinuity: origins, hiding places, and implications for transport

12:10 12:30 Wei Liu Reliable Modeling of Complex Organic/Metal Interfaces

Lunch

Novel spectroscopies in junctions I: conductance, forces and beyond

13:50 14:30 Thomas Wandlowski Charge Transport with Single Molecules: An (Electro-)Chemical Approach

14:30 15:10 Ferdinand Evers

15:10 15:50 Latha Venkataraman Mechanics of Single-Molecule Junctions

Break

Multiscale modelling

16:20 17:00 Joerg Behler Extending the Length and Time Scales of Atomistic Simulations Using Neural Network Potentials

17:00 17:40 Gabor Csanyi Theory and practice of creating first principles-based interatomic potentials

17:40 18:20 Toon Verstraelen ACKS2: Atom-Condensed Kohn-Sham DFT approximated to second order

18:20 19:20 Poster Session 1

Dinner (Authentic Chinese dinner)

Day 2 **15-Oct**

Novel spectroscopies in junctions II: light and voltage-induced dynamics

9:00 9:40 David Masiello Optical- and electron-driven plasmonic environments and their affect upon nearby resonant molecular media

9:40 10:20 Angel Rubio Light-induced dynamical processes in finite and extended systems from TDDFT

Break

10:50 11:30 Tamar Seideman

11:30 12:10 Elke Scheer Transport properties of optically driven molecular switches

12:10 12:50 Volkhard May External Field Control of Sequential Charge Transmission through a Molecular Junction

Lunch

14:00 15:30 Posters session II with coffee

Novel spectroscopies in junctions III: conductance, forces and beyond

15:30 16:10 Misha Galperin Charge and energy transport in molecular junctions

16:10 16:50 Dmitrii E Makarov Mechanically driven quantum transitions: Quantum Zhurkov-Bell Formula

Break

17:10 17:50 Leonhard Grill Voltage-dependent charge transport through single molecular wires

17:50 18:30 José Ignacio Pascual Forces and photons from molecular junctions

Dinner II ("Berlin-style" dinner)

Day 3 **16-Oct**

Simulation of charge transfer in complex environments

9:00 9:40 David Beratan Transport Through Soft, Wet, Fluctuating Biomacromolecules

9:40 10:20 Marcus Elstner Simulation of charge transfer in complex systems

break

Novel spectroscopies in junctions IV: conductance, forces and beyond

10:50 11:30 Joshua Hihath Electromechanical Properties of Atomic and Molecular Junctions

11:30 11:50 Carmen Herrmann Electronic communication through molecular bridges

11:50 12:10 Fatemeh Mirjani Charge transport across insulating self-assembled monolayers

Lunch

Novel spectroscopies in junctions V: inelastic transport, thermoelectrics and Kondo effect

13:40 14:20 Magnus Paulsson Inelastic scattering and conformational change in molecular junctions

14:20 14:40 Alexei Bagrets Kondo effect in binuclear metal-organic molecules on metallic surfaces

14:40 15:00 Jacob Lykkebo Strong Overtones Modes in IETS with Cross-Conjugated Molecules

Break

15:30 16:10 Alessandro Pecchia Current across molecules: pathways, vibrations and heat

16:10 16:50 Gianauelio Cuniberti Carbon thermoelectrics

16:50 17:00 Closing