

New Horizons in materials design
Workshop, 17 – 18 August 2023, Hall 9, MPIE

PROGRAMME

17 August 2023

09:00 – 09:25 Arrival and Registration

09:25 – 9:30 Welcome (Organisers)

Chair: Shyam Katnagallu

09:30 – 10:00 Peter Fratzl (Max Planck Institute of Colloids and Interfaces, Germany)

What natural materials may tell us about sustainable materials design

10:00 – 10:30 Peter Gumbsch (Fraunhofer Institute for Mechanics of Materials, Germany)

Perspectives for programmable materials

10:30 – 11:00 Coffee Break

Chair: Lifang Zhu

11:00 – 11:30 Gabriele Sadowski (TU Dortmund, Germany)

Polymers in pharmaceutical formulations

11:30 – 12:00 Sandra Korte-Kerzel (RWTH Aachen, Germany)

Structural and chemical atomic complexity of lattice defects – From defect phase diagrams to properties of intermetallics

12:00 – 12:30 Christina Scheu (MPIE, Germany)

Designing the functional properties of thermoelectric materials by grain boundary engineering

12:30 – 13:45 Lunch

Chair: Ali Tehrani

13:45 – 14:15 Georg Kresse (Universität Wien, Austria)

Auxiliary Field Quantum Monte Carlo: towards chemical accuracy in solids

14:15 – 14:45 Ralf Drautz (ICAMS, Ruhr Universität Bochum, Germany)

ACE age: applications, generalizations and extensions of the atomic cluster expansion

14:45 – 15:15 Gabor Csányi (University of Cambridge, UK)

TBA

15:15 – 16:00 Coffee Break

Chair: Christoph Freysoldt

16:00 – 16:30 Blazej Grabowski (Universität Stuttgart, Germany)

Anharmonic surfaces in the J_n approximation and beyond

16:30 – 17:00 Martin Friak (Czech Academy of Sciences, Czech Republic)

Theory-guided materials design

17:00 – 17:40 Chris Van de Walle (University of California Santa Barbara, USA)

A New Settler at the Frontier of Materials Design

18:30 Dinner with presentations by Christoph Freysoldt & Mira Todorova

18. August 2023

Chair: Daria Smirnova

09:15 - 09:45 Karsten Reuter (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany)
Out of the crystalline comfort zone - atomistic modelling of operando energy conversion systems

09:45 – 10:15 Axel Groß (Universität Ulm, Germany)
Ion and defects in electrochemical energy conversion and storage

10:15 – 10:45 Coffee Break

Chair: Jing Yang

10:45 – 11:15 Wolf-Gero Schmidt (Universität Paderborn, Germany)
Concerted electron-nuclear motion in phase transitions and exciton transfer

11:15 – 11:45 Liverios Lymperakis (University of Crete, Greece)
Revealing the role of surfaces on the growth and properties of optoelectronic materials through DFT calculations

11:45 – 12:15 Igor Abrikosov (Linköping University, Sweden)
Theory guided design of wide-bandgap semiconductors for the next generation of quantum devices: diamond, silicon carbide and beyond

12:30 – 13:30 Lunch

Chair: Fritz Körmann

13:30 – 14:00 Tilmann Hickel (BAM & MPIE, Germany)
Design of finite temperature materials properties enabled by innovative digital concepts

14:00 – 14:30 Richard Hennig (University of Florida, Gainesville, USA)
Design of AI algorithms for the discovery of novel materials

14:30 – 15:00 Erwin Laure (Max Planck Computing and Data Facility, Germany)
Going to Exascale and beyond - some Myths we should be talking about

15:00 – 15:40 Coffee Break

Chair: Mira Todorova

15:40 – 16:10 Kristina Tschulik (Ruhr Universität Bochum, Germany)
Advancing electrochemical tools to guide the design of better nanocatalysts

16:10 – 16:40 Stefan Wippermann (Philipps-Universität Marburg, Germany)
Novel concepts to simulate reactions at electrified interfaces from first principles

16:40 – 17:10 Dallas Trinkle (University of Illinois, Urbana-Champaign, USA)
Understanding Diffusion in a Complex Concentrated Alloys with Machine Learning and a Variational Principle

17:10 – 17:40 Michael Finnis (Imperial College London, UK)
Diffusion in alumina – recent insights on old problems

17:40 – 17:45 Closing words (Organisers)

18:00 Poster session and BBQ