materials design®

UGM 2025 Vienna, Austria

Scientific Program

Monday, October 6, 2025 Training – Ballroom (ground floor)

9:00 – 17:00 Hands-on *MedeA* software training

18:30 – 21:00 Conference reception

Tuesday, October 7, 2025 All Technical Sessions – Ballroom (ground floor)

9:00 – 9:05 **Erich Wimmer**, Introductory Remarks and Session Chair

9:05 – 9:50 **Ansgar Schäfer**, BASF, Germany: *Quantum Chemistry and Molecular Modeling at BASF*

9:50 – 10:35 **Adrian Sutton FRS**, Imperial College London, UK: *The Ductile-brittle Transition in Metals*

10:35 – 11:00 *Coffee break*

Session Chair: David Reith

11:00– 11:45 **Ivo Koutsaroff,** Akoustis Technologies, USA: *Ab-initio Modeling of Wurtzite AlBScN and Characterization of AlBScN Piezoelectric Thin Film Surface Acoustic Wave Devices Covering 4-8 GHz*

11:45 – 13:30 *Group Photo and Lunch*

Session Chair: Volker Eyert

13:30 – 14:15 **Georg Kresse,** University of Vienna and VASP Software GmbH: *Auxiliary Field Quantum Monte Carlo: Recent Advances and Solids*

14:15 – 15:00 **Ralf Drautz,** Ruhr-University Bochum, Germany, *Foundational Interatomic Potentials with GRACE*

15:00 – 15:30 *Coffee break*

Session Chair: Alexander Mavromaras

15:30 – 16:00 **Kristin Willis** and **Olivier Wagnières,** SICPA, Switzerland: *Accelerating Security Innovation through Materials Simulations at SICPA*

16:00 – 16:30 **Arthur France-Lanord**, University of Paris, Sorbonne: *Kinetics and Thermodynamics of Transformations Using Machine Learning*

17:15 Bus to the conference dinner

18:00 – 22:00 *UGM Reception and Dinner*

Wednesday, October 8, 2025 All Technical Sessions – Ballroom (ground floor)

Session Chair: René Windiks

9:00 – 9:30 **Michele Kotiuga**, Materials Design, *Multiscale Modeling: A Study of Zirconium alloys in Nuclear Reactors*

9:30 – 10:00 **Donald Hlungwani**, University of Limpopo, South Africa, *Evaluation of Promising Solid Electrolyte and Cathode Materials for All-Solid-State-Lithium-Ion Batteries*

10:00 – 10:30: **Marianna Yiannourakou**, Materials Design: *High-Throughput Molecular Simulations for Gas Sorption in Polymers: Automated Workflows for Industrial Material Design*

10:30 – 10:45 *Coffee break*

Session Chair: Garrett Tow

10:45 – 11:15 **Leonid Kahle and Mikael Christensen**, Materials Design**:** *Modeling Interfaces and Microstructures with MedeA*

11:15 – 11:45 **Volker Eyert and Jörg-Rüdiger Hill**, Materials Design: *Generation and Application of Machine-Learned Potentials with MedeA*

11:45 – 12:00 **Clive Freeman,** Materials Design: *Concluding Remarks*

12:00 – 14:00 *Lunch*

14:00 – 17:00 Informal Discussions between MD and Customers

17:00 *Adjourn*