UGM 2019 Vienna

Scientific Program

Wednesday, October 16, 2019:

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

9:05 – 9:50 **Georg Kresse**, University of Vienna, Austria
Organic perovskites: from RPA to phase diagrams via machine learning

9:50 – 10:30 **Moritz to Baben,** GTT, Germany
Assessing phase stability with respect to competing phases

10:30 – 10:50 *Coffee break*

Session Chair: Alexander Mavromaras

10:50 – 11:30 **Antoine Claisse,** Westinghouse, Sweden
Atomistic Modeling at Westinghouse – Needs and Perspectives

11:30 – 12:10 **Richard W. Smith**, Naval Nuclear Laboratory, USA
New Potentials for Zr/H: Collaboration with Materials Design, Inc.

12:10 – 14:00 *Photograph and Lunch*

Session Chair: Volker Eyert

14:00 – 14:20 **Véronique Lachet**, IFP-EN, France
Thermo-physical properties of $U_{1-y}Pu_yO_2$ MOX fuel using classical Monte Carlo simulations

14:20 – 15:00 **Krzysztof Parlinski**, University of Cracow, Poland
Phonon Anharmonicity from ab initio Calculations

15:00 – 15:30 **Stéphane Brice Olou'ou Guifo**, Volkswagen, Germany
Computational design of advanced energy materials for automotive engineering

15:30 – 16:00 *Coffee break*

Session Chair: Clive Freeman

16:00 – 16:40 **Richard Catlow**, Royal Society, UK
Computer Modelling of Nano-Particulate, Microporous, and Photo-active Catalysts

16:40 – 17:20 **James J. P. Stewart**, Stewart Computational Chemistry, USA
A worked example of how Computational Chemistry can help in solving an important and difficult problem

19:00 – 22:00 *UGM Dinner*

Thursday, October 17, 2019:

Session Chair: Dave Rigby

9:00 – 9:20 **Ryan Thomas,** Honeywell, USA
First-Principles Investigation of Hydrogen Trapping in Chemistry Dependent Vacancies of FeCrNi Alloys

9:20 – 9:40 **Wes Everhart**, Honeywell, USA
Applications of DFT to the ductility of intermetallic alloys

9:40 – 10:20 **Marianna Yiannourakou,** Materials Design, France
Predicting and Understanding Properties of Fluids with MedeA

10:20 – 10:40 *Coffee break*

Session Chair: Erich Wimmer

10:40 – 11:20 **Arthur France-Lanord**, MIT, USA
Ion transport in polymer electrolytes: from theory to machine learning

11:20 – 12:30 **Discussion and Conclusions**

12:30 – 14:00 *Lunch*

14:00 – 16:00 Informal Discussions between MD and Customers