Programme

Monday, 3 November 2014

08:15 Pick up at hotels in Jülich

08:45-09:15 Registration

Morning Session (Chair: Martin Müser)

09:15-09:25 Welcome address by **Norbert Attig**, deputy chair JSC

09:25-10:10 **Chandler Becker** (National Institute of Standards and Technology, Gaithersburg, MD, USA):
Facilitating the development, selection, and use of interatomic potentials (force fields) through the development of robust tools and critical comparisons

10:10-10:45 **James Kermode** (King's College London, London, United Kingdom):
Molecular dynamics with on-the-fly machine learning of quantum mechanical forces

10:45-11:15 Coffee break

11:15-12:00 **Peter Brommer** (University of Warwick, Coventry, UK):
Sequential multiscale simulations with *potfit*: First principles data for classical molecular dynamics

12:00-12:30 **Stefan Huber** (Technische Universität München, Garching, Germany):
Towards a physically sound description of zinc oxide (nano-)systems: SCC-DFTB – bridging a gap?

12:30-14:00 Lunch

Afternoon Session (Chair: Toon Verstraelen)

14:00-14:45 **Ralf Drautz** (Ruhr-Universität Bochum, Bochum, Germany):
Bond-Order Potentials: From the electronic structure to million atom simulations

14:45-15:30 **Judith Harrison** (US Naval Academy, Annapolis, USA):
Recent developments and simulations utilizing bond-order potentials

15:30-16:00 Coffee break

16:00-16:30 **Simona Ispas** (Univ. Montpellier 2, Montpellier, France):
A structural fitting approach to develop effective potentials from *ab initio* simulations of amorphous systems

16:30-17:00 **Martin Gren** (Chalmers Uni. of Technology, Gothenburg, Sweden):
Study of grain boundary deformation mechanisms in cemented carbides using a model potential for the W-C-Co system

17:00-17:30	Poster power presentations 1-slide, ≈2-minute presentation of each poster
17:30-18:00	Group photo and poster session start
18:00-19:30	Welcome reception with poster session
19:30	Bus to hotels in Jülich

Tuesday, 4 November 2014

08:15 Pick up at hotels in Jülich

Morning Session (Chair: Lars Pastewka)

08:45-09:30 **Mathieu Salanne** (University Pierre and Marie Curie, Paris, France):
Building polarizable force fields for ionic materials and liquids

09:30-10:15 **Ellad Tadmor** (University of Minnesota, Minneapolis, MN, USA):
OpenKIM and the future of force fields: Citability, portability and transferability

10:15-10:45 **Konstantin Smirnov** (CNRS - University Lille 1, Villeneuve d'Ascq, France):
Critical assessment of SQE model for the development of polarizable force fields

10:45-11:15 Coffee break

11:15-12:00 **Adri van Duin** (Penn State, University Park, USA):
Applications of ReaxFF to complex materials and material interfaces

12:00-12:30 **Michal H. Kolar** (Forschungszentrum Jülich, Jülich, Germany):
Halogen bonds, sigma-holes and molecular mechanics of modern drug candidates

12:30-14:00 Lunch

Afternoon Session (Chair: Konstantin Smirnov)

14:00-14:45 **Karsten Albe** (TU Darmstadt, Darmstadt, Germany):
Tersoff-Abell type bond-order potentials: A review

14:45-15:30 **Sandro Scandolo** (ICTP, Trieste, Italy):
Polarizable force-fields for oxides (including water)

15:30-16:00 Coffee break

16:00-16:30 **Wolf Dapp** (Forschungszentrum Jülich, Jülich, Germany):
Force-field based modeling of redox reactions

16:30-17:15 **Rochus Schmid** (Ruhr-University Bochum, Bochum, Germany):
First principles parametrized force fields for porous coordination polymers and related systems: Development and application

17:15-17:45 **Toon Verstraelen** (Ghent University, Zwijnaarde, Belgium):
How to ensure the accuracy of polarizable force fields?

17:45-18:30 Poster session and discussion

Evening

18:30 Bus to dinner at Castle Obbendorf (Hambach)

18:45 Workshop dinner

21:30 Bus to hotels in Jülich

Wednesday, 5 November 2014

08:15 Pick up at hotels in Jülich

Morning Session (Chair: Martin Müser)

08:45-09:30 **Wojciech Szlachta** (University of Cambridge, Cambridge, United Kingdom):
Accuracy and transferability of GAP models for tungsten

09:30-10:00 **Ming Hu** (RWTH Aachen University, Aachen, Germany):
Thermal transport in two-dimensional silicon calls for accurate force field

10:00-10:30 **Lars Pastewka** (Fraunhofer IWM, Freiburg, Germany):
Screened empirical bond-order potential for Si-C-H

10:30-11:00 Coffee break

11:00-11:30 **Alejandro Strachan** (Purdue University, West Lafayette, USA):
Reactive MD simulations: From nanoscale electrochemistry to detonation initiation

11:30-12:00 **Jari Jalkanen** (Forschungszentrum Jülich, Jülich, Germany):
Systematic analysis and extension of embedded atom models

12:00-12:30 **Paul Popelier** (University of Manchester, Manchester, Great Britain):
Quantum Chemical Topology: Towards a novel protein force field with polarisable multipolar electrostatics

12:30-12:35 Closing remarks

12:45 Lunch at Forschungszentrum Jülich, or alternatively, departure to Cologne train station / brewery (drinks and food on one's own expense), arrival in Cologne at around 13:45