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ZERMATT
MATTERHORN

Probing Potential Energy Surfaces PPES-IV

April 10-15, 2016
Zermatt
Switzerland

Program

Sunday, April 10

18:00 - 19:30	Dinner	
Session 1: Materials big data, the concepts, infrastructure and applications (Chair: Matthias Scheffler)		
20:00 - 20:30	Matthias Scheffler	Welcome address and The NOMAD Idea
20:30 - 21:00	Fawzi Mohamed	Building a code independent database
21:00 - 21:30	Emre Ahmetcik	Machine learning of the stability of octet binaries

Monday, April 11

Session 1: Materials big data, the concepts, infrastructure and applications, cont. (Chair: Matthias Rupp)		
08:30 - 09:00	Georg Huhs	The NOMAD Encyclopedia
09:00 - 09:30	Johan M. Carlsson	Materials simulation in industry
09:30 - 10:00	Hagen-Henrik Kowalski	First-principle study of thermoelectric magnesium silicides with high-throughput techniques
Session 2: Electron-phonon coupling (Chair: Igor Ying Zhang)		
10:00 - 10:30	Stefan K. Estreicher	Phonons and defects in semiconductors: Beyond the phonon-scattering assumption
10:30 - 11:00	Christian Carbogno	Electron-phonon coupling
11:00 - 18:00		Hands on sessions and group discussion
18:00- 19:30	Dinner	
Session 3: Semiconductor / photovoltaics and excited states (Chair: Christian Carbogno)		
20:00 - 20:30	Claudia Draxl	Opto-electronic excitations at interfaces between low-dimensional materials
20:30 - 21:00	Friedhelm Bechstedt	Topological surface and interface states from first principles
21:00 - 21:30	Axel Groß	Modelling the electrochemical environment in electrocatalytic devices

Tuesday, April 12

Session 4: (Bio)molecules and water (Chair: Sergey Levchenko)		
08:30 - 09:00	Roberto Car	The role of exchange and correlations
09:00 - 09:30	Carsten Baldauf	Complex carbohydrates are a challenge for molecular simulations
09:30 - 10:00	Mariana Rossi	Nuclear quantum effects
10:00 - 18:00		Hands on sessions and group discussion
18:00 - 19:30	Dinner	
Session 5: Basic concepts (Chair: Claudia Draxl)		
20:00 - 20:30	Xiangyue Liu	Numerical convergence of advanced electronic correlation methods for accurate cohesive properties in materials science
20:30 - 21:00	Björn Bieniek	Numerical quality control in computational materials databases

Wednesday, April 13

Session 5: Basic concepts, cont. (Chair: Claudia Draxl)		
08:30 - 09:00	Karsten Reuter	Exothermic surface reactions: Disentangling phononic and electronic energy dissipation
09:00 - 09:30	Niklas Menzel	Compressed sensing approach to select accurate atom-centered basis functions for DFT and MP2 calculations
09:30 - 10:00	Matthias Rupp	Machine learning models for quantum mechanics
10:00 - 10:30	Sebastian Kokott	Assessment of the accuracy of hybrid density functionals for polarons in oxides
10:30 - 18:00		Hands on sessions and group discussion
18:00 - 19:30	Dinner	
Session 5: Basic concepts, cont. (Chair: Mariana Rossi)		
20:00 - 20:30	Igor Ying Zhang	A test set for materials science and engineering
20:30 - 21:00	Tonghao Shen	Coupled cluster theory for periodic systems
21:00 - 21:30	Christopher Sutton	An accurate description of excited state energies in organic semiconductors using the random phase approximation

Thursday, April 14

Session 7: Surfaces: nanostructures and catalysis (Chair: Karsten Reuter)		
08:30 - 09:00	Harald Brune	Magnetic Remanence in Single Atoms
09:00 - 09:30	Christian Ratsch	A new approach to calculate the surface energy for a polar system
09:30 - 10:00	Bryan Goldsmith	Disintegration and redispersion of noble metal nanoparticles: an ab initio thermodynamics study
10:00 - 10:30	Karl-Heinz Ernst	Non-planar aromatic hydrocarbons and metal surfaces: Is there any reasonable prediction of lateral interactions or binding sites?
10:30 - 11:00	Hong Li	Polarity inversion in GaN nanostructures
11:00 - 18:00		Hands on sessions and group discussion
19:00 - 23:00	Conference dinner	

Friday, April 15

Session 8: Surfaces: nanostructures and catalysis, cont. (Chair: Carsten Baldauf)		
09:30 - 10:00	Weiqi Wang	Role of spin states at finite temperature in oxygen adsorption and activation on noble-metal clusters
10:00 - 10:30	Sergey Levchenko	Defects at surfaces