

Theory and Computation for Interface Science and Catalysis: Fundamentals, Research and Hands on Engagement using VASP

Report of Contributions

Contribution ID: 1

Type: **not specified**

Check-In, Lap-Top Registration and Informal Dinner

Sunday 2 November 2014 04:00 (3 hours)

Contribution ID: 2

Type: **not specified**

Energy Materials Challenges, Cynthia Friend, Harvard

Monday 3 November 2014 09:15 (45 minutes)

Contribution ID: 3

Type: **not specified**

Introduction to Pseudopotentials and Electronic Structure, Phil Allen, Stony Brook University

Monday 3 November 2014 10:30 (45 minutes)

Contribution ID: 4

Type: **not specified**

Introduction to Density Functional Theory, Deyu Lu, BNL

Monday 3 November 2014 11:15 (45 minutes)

Contribution ID: 5

Type: **not specified**

Lunch – Berkner

Monday 3 November 2014 12:00 (1h 30m)

Contribution ID: 6

Type: **not specified**

Tutorial 1: Intro to Vasp Calculations for Solids, Martijn Marsman, U.Wien

Monday 3 November 2014 13:30 (1h 30m)

Contribution ID: 7

Type: **not specified**

Tutorial 2: Intro to Vasp Calculations for Surfaces, Martijn Marsman, U. Wien

Monday 3 November 2014 15:30 (1h 30m)

Contribution ID: 8

Type: **not specified**

Dinner – Berkner

Monday 3 November 2014 17:00 (1h 30m)

Contribution ID: 9

Type: **not specified**

Welcome & Overview, Mark Hybertsen, BNL

Monday 3 November 2014 08:30 (45 minutes)

Contribution ID: **10**

Type: **not specified**

Model catalyst studies: Design principles, Jose Rodriguez, BNL

Tuesday 4 November 2014 08:30 (45 minutes)

Contribution ID: 11

Type: **not specified**

Emerging In-Situ Experimental Capabilities in Surface Science at the CFN, Anibal Boscoboinik, BNL

Tuesday 4 November 2014 09:15 (45 minutes)

Contribution ID: 12

Type: **not specified**

DFT for Heterogeneous Catalysis, Ping Liu, BNL

Tuesday 4 November 2014 10:30 (45 minutes)

Contribution ID: 13

Type: **not specified**

Modeling Reaction Pathways, Dion Vlachos, Univ. Delaware

Tuesday 4 November 2014 11:15 (45 minutes)

Contribution ID: **14**

Type: **not specified**

Lunch – Berkner

Tuesday 4 November 2014 12:00 (1h 30m)

Contribution ID: 15

Type: **not specified**

Tutorial 3: Vasp Calculations for Reaction Pathways, Wei An, BNL

Tuesday 4 November 2014 13:30 (1h 30m)

Contribution ID: 16

Type: **not specified**

Tutorial 4: Tools for Kinetic Modeling, Alexander Mironenko, Univ. Delaware

Tuesday 4 November 2014 15:30 (1h 30m)

Contribution ID: 17

Type: **not specified**

Dinner – Berkner

Tuesday 4 November 2014 17:00 (1h 30m)

Contribution ID: **18**

Type: **not specified**

Analysis of Core Level Spectra, Mark Hybertsen, BNL

Wednesday 5 November 2014 09:01 (44 minutes)

Contribution ID: 19

Type: **not specified**

Probing Catalyst-Support Interactions Using a Combination of Experiment and Theory, Michael White, BNL & Stony Brook Univ.

Wednesday 5 November 2014 09:45 (45 minutes)

Contribution ID: 20

Type: **not specified**

Catalyst Design with DFT, Jinguang Chen, Columbia & BNL

Wednesday 5 November 2014 11:00 (45 minutes)

Contribution ID: 21

Type: **not specified**

Introduction to PAW for Electronic Structure, Martijn Marsman, U. Wien

Wednesday 5 November 2014 11:45 (30 minutes)

Contribution ID: 22

Type: **not specified**

Lunch – Berkner

Wednesday 5 November 2014 12:15 (1h 15m)

Contribution ID: 24

Type: **not specified**

Tutorial 5: Vasp Calculations for Electronic Properties and Probes of Core Levels, Mark Hybertsen, BNL

Wednesday 5 November 2014 13:30 (1h 30m)

Contribution ID: 25

Type: **not specified**

Break-Out Time for Informal Discussions

Wednesday 5 November 2014 15:30 (1h 30m)

Contribution ID: 26

Type: **not specified**

Dinner – Atlantis Aquarium, Riverhead, NY

Wednesday 5 November 2014 17:00 (3 hours)

Contribution ID: 27

Type: **not specified**

Materials for photocatalysis, Peter Khalifah, BNL & SBU

Thursday 6 November 2014 08:46 (44 minutes)

Contribution ID: 28

Type: **not specified**

Transmission electron microscopy in atmospheric pressure liquids and gases, Eric Stach, BNL

Thursday 6 November 2014 09:30 (45 minutes)

Contribution ID: 29

Type: **not specified**

TiO₂-Water Interface Properties, Annabella Selloni, Princeton

Thursday 6 November 2014 10:45 (45 minutes)

Contribution ID: **30**

Type: **not specified**

Photocatalytic Water Oxidation at the GaN-Water Interface, James Muckerman, BNL

Thursday 6 November 2014 11:30 (45 minutes)

Contribution ID: **31**

Type: **not specified**

Lunch – Berkner

Thursday 6 November 2014 12:15 (1h 30m)

Contribution ID: 32

Type: **not specified**

Tutorial 6: Vasp Calculations for Ab Initio Molecular Dynamics, Deyu Lu, BNL

Thursday 6 November 2014 13:45 (1h 30m)

Contribution ID: 33

Type: **not specified**

Tutorial 7: Vasp Calculations With Model Solvation, Neerav Kharche, BNL

Thursday 6 November 2014 15:45 (1h 30m)

Contribution ID: **34**

Type: **not specified**

Dinner – Berkner

Thursday 6 November 2014 18:00 (1h 30m)

Contribution ID: 35

Type: **not specified**

Materials discovery for catalysis, Thomas Bligaard, SLAC

Friday 7 November 2014 09:00 (1 hour)

Contribution ID: 36

Type: **not specified**

Evolutionary Algorithms for Structure Discovery, Artem Oganov, Stony Brook Univ.

Friday 7 November 2014 10:30 (1h 30m)

Contribution ID: 37

Type: **not specified**

Lunch – Berkner

Friday 7 November 2014 12:00 (1h 30m)

Contribution ID: **38**

Type: **not specified**

Tutorial 8: Intro to USPEX, Oganov Group

Friday 7 November 2014 13:30 (2 hours)

Contribution ID: 39

Type: **not specified**

Breakfast

Monday 3 November 2014 08:15 (14 minutes)

Contribution ID: 40

Type: **not specified**

Breakfast

Tuesday 4 November 2014 08:15 (14 minutes)

Contribution ID: 41

Type: **not specified**

Breakfast

Wednesday 5 November 2014 08:45 (15 minutes)

Contribution ID: 42

Type: **not specified**

Breakfast

Thursday 6 November 2014 08:30 (15 minutes)

Contribution ID: 43

Type: **not specified**

Breakfast

Friday 7 November 2014 08:30 (29 minutes)