

ICMR workshop
“*Ab-initio description of charged systems and solid/liquid interfaces for
semiconductors and electrochemisty*”

PROGRAMME

SUNDAY, July 6, 2015

6:00 – 8:00 pm **Registration and Welcome Reception**

MONDAY, July 7, 2014

7:30 – 8:30 am *Breakfast*

9:00 – 9:10 am **Opening Remarks**

Morning session: Points Defects in Semiconductors

9:10 – 10:10 am **Alfredo Pasquarello (EPFL, Switzerland)**
Accurate modelling of defect levels

10:10 – 11:10 am **Fabien Bruneval (France)**
Recent methodological advances in the calculation of charged
point defects

11:10 – 11:30 am *Coffee Break*

11:30 – 12:30 am **Christoph Freysoldt (MPIE, Germany)**
Point defects in supercells: Correction schemes to describe the
dilute limit

12:45 – 2:00 pm *Lunch*

Afternoon session: Solvation models

2:00 – 3:00 pm **Tomas A. Arias (Cornell University, USA)**
Joint density-functional theory: a predictive, ab initio description
of the electrochemical interface

3:00 – 4:00 pm **Donald Truhlar (University of Minnesota, USA)**
Solvation models in quantum chemistry

4:00 – 4:25 pm *Coffee Break*

4:25 – 4:45 pm **Kiran Mathew (Cornell University, USA)**
Solid/liquid interfaces in DFT: Implementation in VASP

4:45 – 5:05 pm **Giuseppe Fiscaro (University of Basel, Switzerland)**
Particle-particle interaction and space-dependent effective
dielectric constant in colloidal system

5:05 – 6:15 pm **Flash Poster Presentation**

6:30 pm *Dinner*

TUESDAY, July 8, 2014

7:30 – 8:30 am *Breakfast*

Morning session: Electrochemistry - modelling

9:00 – 10:00 am **Michiel Sprik (Cambridge, UK)**
All atom density functional simulation of metal oxide-water interfaces

10:00 – 11:00 am **Minoru Otani (Japan)**
First-principles molecular dynamics study of electrochemical reactions at electrode-electrolyte interfaces

11:00 – 11:30 am *Coffee Break*

11:30 – 12:30 pm **Mira Todorova (MPIE, Germany)**
Connecting defect chemistry in semiconductors and electrochemistry

12:45 – 3:10 pm *Lunch*

Afternoon session

3:10 – 3:30 pm **Vladan Stevanovic (Colorado School of Mines & NREL, USA)**
Assessing the capability of semiconductors to split water using Ionization Potentials and Electron Affinities only

3:30 – 3:50 pm **Hartwin Peelaers (UCSB, USA)**
Polarons in thin Ga₂O₃ layers

3:50 – 4:15 pm *Coffee Break*

Surfaces and Interfaces

4:15 – 5:15 pm **Axel Groß (Universität Ulm, Germany)**
Toward a more realistic modelling of the electrochemical double layer at metal electrodes

5:15 – 6:15 pm **Adam Foster (Aalto University, Finland)**
Probing solid-liquid interfaces at the atomic scale

6:30 pm *Dinner*

WEDNESDAY, July 9, 2014

7:30 – 8:30 am *Breakfast*

Morning session: Oxides

9:00 – 10:00 am **Mike Finnis (Imperial, UK)**
Defect chemistry in oxide scales

10:00 – 11:00 am **Anderson Janotti (UCSB, USA)**
Small polarons in the bulk and on the surface of transition-metal oxides

11:00 – 11:30am *Coffee Break*

11:30 – 12:30 am **Patrick Rinke (FHI, Germany)**
Space charge transfer in organic/inorganic hybrids

12:45 – 2:00 pm *Lunch*

Afternoon session: Low dimensional materials

2:00 – 3:00 pm **Nithaya Chetty (Univ Pretoria, South Africa)**
Defects and interfaces/interlines in 2D materials

3:00 – 6:00 pm **Poster Session**

6:30 pm *Conference Dinner (Off campus dinner)*

THURSDAY, July 10, 2014

7:30 – 8:30 am *Breakfast*

Morning session: Spectroscopy in Water – theory and experiment

9:00 – 10:00 am **Giulia Galli (UC Davis, USA)**
Electronic properties of aqueous interfaces: coupled ab initio
molecular dynamics and GW calculations

10:00 – 11:00 am **Marie Gaigeot (Universite d'Evry, Paris, France)**
Simulating vibrational spectra at solid-liquid interfaces, including
electrolytes, with DFT-based MD simulations

11:00 – 11:30 am *Coffee Break*

11:30 – 12:30 am **Heather Allen (Ohio State, USA)**
Electric fields at the air/water interface: Water, ions, and lipids

12:30 – 12:50 pm **Das Pemmaraju (Lawrence Berkeley National Lab, USA)**
Charged supercell calculations for modelling X-ray photoemission
spectra

1:00 – 3:00 pm *Lunch*

Afternoon session: Ions in Water

3:00 – 4:00 pm **Eckhard Spohr (Universität Essen-Duisburg, Germany)**
Modelling proton discharge with reactive force fields

4:00 – 4:25 am *Coffee Break*

4:25 – 4:45 pm **A. Marco Saita (Sorbonne Universités Paris, France)**
Proton-hopping in water and solutions under intense electric fields

4:45 – 5:05 am **Oleg A. Borodin (Army Research Laboratory, USA)**
Molecular dynamics simulations of the lithium transport through
solid electrolyte interphase (SEI) components and SEI-electrolyte
interface

5:05 – 5:25 pm **Johannes Frenzel (Bochum University, Germany)**
Methanol synthesis from molecular dynamics

5:25 – 5:45 pm **Brandon C. Wood (Lawrence Livermore NL, USA)**
Chemistry and transport at semiconductor-water interfaces for photoelectrochemical water splitting

6:00 pm *Dinner (BBQ at Goleta Beach)*

FRIDAY, July 11, 2014

7:30 – 8:30 am *Breakfast*

Morning session: Solid/Liquid interface and Double Layer

9:00 – 10:00 am **Marcus Valtiner (MPIE, Germany)**
Force probe experiments to elucidate structure and dynamics at electrified and hydrated interfaces

10:00 – 10:20 pm **De-en Jiang (University of California, Riverside, USA)**
Understanding electric double-layer capacitors

10:20 – 10:40 am *Coffee Break*

10:40 – 11:00 am **T. J. Mills (University of Oregon, USA)**
Theory and simulations of electrocatalyst-coated semiconductor electrodes for solar water splitting

Corrosion

11:00 – 12:00 noon **Ivan Cole (SCIRO, Australia)**
Atmospheric corrosion

12:30 pm *Lunch*