

# Program

## Sunday, 8 December 2019

- 16:00 – 19:00    Registration
- 18:00            *BUFFET SUPPER and get-together*
- 19:15 – 20:15    R. Kramer Campen    **Towards a femtosecond resolved view of the hydrogen evolution reaction on Au and Pt**

## Monday, 9 December 2019

- 08:00            *BREAKFAST*
- 08:45 – 09:00    Scientific organizers    **Welcome words**
- 09:00 – 10:00    Ulrike Diebold            **Bridging ultrahigh vacuum surface science and liquid water: First steps and future opportunities**
- 10:00 – 10:45    Mira Todorova            **Predicting atomic structure and chemical reactions at solid-liquid interfaces by first principles**
- 10:45 – 11:15    *COFFEE BREAK*
- 11:15 – 12:00    Fabiola Dominguez Flores    **Interaction of ions across carbon nanotubes**
- 12:00 – 12:45    Karla Banjac              **Emergence of potential-controlled Cu nanocubes under *operando* CO<sub>2</sub> reduction**
- 12:45            *LUNCH / networking*

# Program

Monday, 9 December 2019

14:45 – 15:30	Marc Koper	<b>Electrochemical surface science of platinum</b>
15:30 – 16:15	Henrik Kristoffersen	<b>Modeling the liquid water-Pt(111) interface</b>
16:15 – 16:45	<i>COFFEE BREAK</i>	
16:45 – 17:30	Leon Jacobse	<b>Operando surface structure determination of Pt(111) under realistic oxygen reduction conditions using high-energy surface X-ray diffraction</b>
17:30-18:15	Jinggang Lan	<b>Ionization of water as an effect of quantum delocalization at aqueous electrode interfaces</b>
18:30	<i>DINNER</i>	
19:30	<b>Posterflash (1 min.) and postersession (<u>even numbers</u>)</b>	

# Program

**Tuesday, 10 December, 2019**

08:00	<i>BREAKFAST</i>	
09:00 – 09:45	Aliaksandr Bandarenka	<b>Why electrolytes can significantly control the catalytic activity. An experimental approach</b>
09:45 – 10:30	Jan Rossmeisl	<b>Electrocatalysis at the atomic scale</b>
10:30 – 11:00	<i>COFFEE BREAK</i>	
11:00 – 11:45	Kristina Tschulik	<b>Electrochemical studies of nanoparticle observed with dark-field microscopy</b>
11:45 – 12:30	Karsten Reuter	<b>On the active site model in computational catalyst screening</b>
12:30 – 12:40	<i>Conference Photo (in the front of the lecture hall)</i>	
12:40	<i>LUNCH / networking</i>	
14:30	<b>Excursion: Wine tasting at the winery Broel</b>	
18:15	<i>DINNER</i>	
19:15 – 20:15	Daniel A. Scherson	<b>Electrode stimulation</b>

# Program

Wednesday, 11 December, 2019

08:00	<i>BREAKFAST</i>	
08:45 – 09:45	Elena Savinova	<b>Operando FTIR investigation of borohydride electrooxidation on nickel</b>
09:45 – 10:30	Stijn Mertens	<b>Electrochemical orbital imaging</b>
10:30 – 11:00	<i>COFFEE BREAK</i>	
11:00 – 11:45	Markus Valtiner	<b>Angstrom-resolved characterization of electrochemical interfaces in real time during polarization</b>
11:45 – 12:30	Jun Cheng	<b>Ab initio modeling of electric double layers on single crystal electrodes</b>
12:30	<i>LUNCH / networking</i>	
14:45 – 15:30	Clotilde Cucinotta	<b>Improving the design of electrochemical materials and devices with theory and modelling</b>
15:30 – 16:15	Bridget Murphy	<b>Investigating atomic scale structure and kinetics of liquid metal–electrolyte interfaces</b>
16:15 – 16:45	<i>COFFEE BREAK</i>	
16:45 – 17:30	Vivek Sinha	<b>Towards multiscale modelling of the semiconductor electrolyte interface for oxygen evolution reaction</b>
17:30-18:15	Celine Merlet	<b>Exploring the properties of concentrated electrolyte / electrode interfaces in supercapacitors using idealised coarse-grained models</b>
18:30	<i>DINNER</i>	
19:30	<b>Posterflash (1 min.) and postersession (<u>odd numbers</u>)</b>	

# Program

Thursday, 12 December, 2019

08:00	<i>BREAKFAST</i>	
08:45 – 09:00	<b>Poster awards</b>	
09:00 – 09:45	Marcella Iannuzzi	<b>Interfaces by ab initio molecular dynamics</b>
09:45 – 10:30	Olga Sambalova	<b>Magneto-optical Kerr effect set-up for operando probing of electrode surfaces</b>
10:30 – 11:00	<i>COFFEE BREAK</i>	
11:00 – 11:45	Izabella Brand	<b>Investigating molecular scale changes at the electrode-electrolyte interface using polarization modulation infrared reflection absorption spectroscopy</b>
11:45 – 12:30	David Fermin	<b>Oxygen electrocatalysis at transition metal oxide nanostructures</b>
12:30	<i>LUNCH / networking</i>	
14:45 – 16:15	<b>Round table</b>	<b>Challenges and opportunities of solid/liquid operando surface science: method development, key applications and interdisciplinarity</b>
16:15 – 16:45	<i>COFFEE BREAK</i>	
16:45 – 17:30	Ismael Pérez Díez	<b>Mapping charge transport at electrode/liquid interfaces: from oxides films to biomolecules</b>
17:30-18:15	Ali Ismael	<b>Tuning the thermoelectric performance of aromatic molecules</b>
18:30	<i>HERAEUS DINNER</i> <i>(social event with cold &amp; warm buffet with complimentary drinks)</i>	

# Program

Friday, 13 December, 2019

08:00	<i>BREAKFAST</i>	
09:00 – 09:45	Harald Oberhofer	<b>Parametrizing implicit solvation models</b>
09:45 – 10:30	Manon Bertram	<b>Adsorbate properties on atomically-defined <math>\text{Co}_3\text{O}_4(111)</math> in UHV and the electrochemical environment</b>
10:30 – 11:00	<i>COFFEE BREAK</i>	
11:00 – 11:45	Andreas Erbe	<b>Probing water and surface oxides on electrodes by coupling in situ spectroscopic techniques</b>
11:45– 12:20	<b>Brainstorming</b>	
12:20 – 12:30	Scientific organizers	<b>Closing words</b>
12:30	<i>LUNCH</i>	

**End of the seminar and departure**

*NO DINNER for participants leaving on Saturday morning*