



Workshop Molecular Approaches to Heterogeneous Catalysis and Electrocatalysts

November 20-21, 2017

Organizing Committee

Suljo Linic (TUM-IAS Hans Fischer Fellow, University of Michigan, USA)

Karsten Reuter (TUM)

Technical University of Munich · Institute for Advanced Study
Lichtenbergstraße 2 a · 85748 Garching · Germany

Program

MONDAY, NOVEMBER 20, 2017

Auditorium (ground floor)

1:00 – 1:15 p.m.	Welcome Address Ernst Rank (Director, TUM-IAS)
1:15 – 1:50 p.m.	Technical analysis of the CO₂ emission impact and catalytic strategies for addressing the problem Suljo Linic (TUM-IAS Hans Fischer Fellow, University of Michigan)
1:50 – 2:25 p.m.	Catalysis for light alkanes – from methane functionalization to light olefins Johannes A. Lercher (TUM)
2:25 – 3:00 p.m.	Biomass conversion to fuels and chemicals Will Medlin (University of Colorado Boulder)
3:00 – 3:30 p.m.	<i>Coffee Break (Foyer, ground floor)</i>
3:30 – 4:05 p.m.	Introduction to electrocatalysis Michael Janik (Pennsylvania State University)
4:05 – 4:40 p.m.	Surface science and X-ray synchrotron methods applied to catalysis Beatriz Roldan Cuenya (Fritz-Haber Institute of Max Planck Society)
4:40 – 5:15 p.m.	Catalysis of clusters in the non-scalable size regime I Ulrich Heiz (TUM)
5:15 – 5:50 p.m.	Multiscale modeling of catalysis Karsten Reuter (TUM)

TUESDAY, NOVEMBER 21, 2017

Auditorium (ground floor)

- 8:30 – 9:05 a.m. ***Operando* nanocatalysis: size, shape, composition, and chemical state effects**
Beatriz Roldan Cuenya (Fritz-Haber Institute of Max Planck Society)
- 9:05 – 9:40 a.m. **Catalysis of clusters in the non-scalable size regime II**
Ulrich Heiz (TUM)
- 9:40 – 10:15 a.m. **Refining first-principles photo-electrocatalysis**
Karsten Reuter (TUM)
- 10:15 – 10:45 a.m. *Coffee Break (Foyer, ground floor)*
- 10:45 – 11:20 a.m. **Organic monolayers in heterogeneous catalysis: how “crowding” the reactants can improve catalyst specificity**
Will Medlin (University of Colorado Boulder)
- 11:20 – 11:55 a.m. **Lessons from enzymes - On the role of steric constraints and chemical environments for catalysis**
Johannes A. Lercher (TUM)
- 11:55 – 12:30 p.m. **Development of electrocatalytic materials guided by computational chemistry: fuel cells and electrolysis**
Michael Janik (Pennsylvania State University)
- 12:30 – 13:05 p.m. **Maximizing efficiencies of photocatalytic water splitting by engineering interfaces in multi-component photocatalysts**
Suljo Linic (TUM-IAS Hans Fischer Fellow, University of Michigan)