



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)

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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. *Coffee Break (Foyer, ground floor)*
- 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. **Catalysis for light alkanes – from methane functionalization to light olefins**
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)