

# Einladung

## zur Verleihung des Loschmidt-Preises 2015 der Chemisch-Physikalischen Gesellschaft

an  
**Dr. Zbynek Novotny**  
und  
**Dr. Martin Richter**

**am Dienstag, 19. Jänner 2016, um 17:30 Uhr**

**Ort: Lise-Meitner-Hörsaal, Universität Wien, Fakultät für Physik  
1090 Wien, Strudlhofgasse 4/Boltzmannngasse 5, 1. Stock**

*Treppenfrier Zugang: Boltzmannngasse 5, Lift, 1. Stock rechts über den Gang zum Hintereingang des Hörsaals*

**sowie zu den Preisvorträgen**

**Dr. Zbynek Novotny**

### **The Reconstructed $\text{Fe}_3\text{O}_4(001)$ Surface as an Adsorption Template**

Single atoms anchored to metal oxides offer great potential for achieving high activity and selectivity in heterogeneous catalysis. Unfortunately, supported metal atoms are generally not stable and tend to agglomerate to clusters already at fairly low temperatures ( $<300$  K). In this talk, I will demonstrate the key findings from my graduate research: a discovery of a unique adsorption properties of the  $\text{Fe}_3\text{O}_4(001)-(\sqrt{2}\times\sqrt{2})$  surface and its ability to stabilize single metal atoms at temperatures as high as 700 K. The properties of single atoms of Fe, Au and Pd will be discussed. Finally, I will present a brief highlight of my current research at PNNL.

**Dr. Martin Richter**

### **Semiclassical Molecular Dynamics - A Modern Way to Connect Theory to Time-Resolved Experiments**

Semiclassical molecular dynamics (MD) simulations have become an indispensable tool for the investigation of photoinduced processes in molecular systems and can be used to follow femtosecond non-adiabatic relaxation processes in real time. Exemplarily, the ultrafast relaxation dynamics of pyrimidine nucleobases after UV excitation is presented. The combination of microscopic MD results with state of the art spectra simulation methodologies is discussed.

**Im Anschluss an die Veranstaltung bitten wir zu einem kleinen Buffet**

**Mit freundlicher Unterstützung der Kulturabteilung der Stadt Wien - Wissenschafts- und  
Forschungsförderung**

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