



UNIVERSITÄT
LEIPZIG

Fakultät für Chemie und Mineralogie

Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie

08.11.2018

Einladung zum Wilhelm-Ostwald-Institutskolloquium

Am **Montag, dem 10.12.2018, 16:15 Uhr**, spricht

Prof. Sandra Luber

Institut für Chemie, Universität Zürich, Zürich, Schweiz

im Wislicenus-Hörsaal, Johannisallee 29, 04103 Leipzig

zum Thema:

Advanced Computational Methods for Spectroscopy and Catalysis

Abstract

I will give an overview about our work for the development of computational approaches with emphasis on spectroscopy, catalysis, and informed design. Recently, we have especially focused on the improved description of condensed phase systems via forefront methods such as high-performance *ab initio* molecular dynamics (AIMD).

We have, for instance, presented computationally efficient approaches for the calculation of Raman spectra for periodic systems as well as first AIMD spectra for vibrational Raman optical activity, enabling now a dynamic, accurate description of chiral systems. Interfaces are also of high interest, and pioneering studies have been carried out for sum frequency generation spectroscopy from semiconductor surface via AIMD. In addition, efficient methods - based on, e.g., periodic density functional theory embedding – for the analysis of complex systems have been developed.

Other research directions have concerned the study of functional systems, in particular for catalysis. In close collaboration with experimental groups, we have worked on solar light-driven water splitting for sustainable hydrogen production where we have presented some of the rare active water oxidation catalysts closely mimicking nature's photosystem II. Computational advances include calculation of properties, reaction mechanisms and networks as well as improved inclusion of environmental and solvent effects. This has paved the way for highly sought-after structure-activity relationships and informed *in silico* design of novel efficient and stable catalysts.

Ab 15:30 Uhr findet ein gemeinsames Kaffeetrinken in Raum 410 (TA) statt.