

## Methods in Molecular Energy Research: Theory and Spectroscopy

August 30 - September 4, 2015

Wissenschaftspark Gelsenkirchen, Germany

Combining spectroscopic methods with theoretical chemistry has evolved into a major and powerful component of modern research in molecular sciences. This summer school aims to offer students, postdocs and young researchers the necessary knowledge to bridge the gap between these two approaches.

The school consists of morning lectures by international experts, in which various spectroscopic techniques are presented and the basics of the computational approaches are discussed. Every afternoon, practical sessions will then focus on electronic structure calculations and the prediction of spectroscopic properties.

### Keynote speakers:



- William Tolman  
University of Minnesota



- Stefan Grimme  
University of Bonn

### Lecturers:

- Thorsten Glaser
- Felix Tuczek
- Frank Neese
- Eckhard Bill
- Serena DeBeer
- Maurice van Gastel

### Topics

- Introduction to computational chemistry
- Ligand field theory, Magnetism
- Electron paramagnetic resonance (EPR), optical (UV/Vis) and MCD, vibrational (IR/Raman), Mössbauer, and X-ray spectroscopies (XAS, XES)
- Calculation of spectroscopic parameters
- Advanced special interest lectures



### Organizers:

Dimitrios Pantazis, Dimitrios Manganas, Eckhard Bill  
Max Planck Institute for Chemical Energy Conversion

<http://www.cec.mpg.de/workshops/summerschool2015>

This Summer School is also the kick-off event for the International Max Planck Research School on Reactive Structure Analysis for Chemical Reactions (IMPRS RECHARGE)

