

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>