

Electronic Structure and Spectroscopy of Transition Metal Complexes

September 29 - October 4, 2019

Wissenschaftspark Gelsenkirchen, Germany

The school is addressed to graduate students, post-doctoral scientists, and senior researchers with either experimental (synthetic/spectroscopic) or theoretical background, who are interested in the deep connections between molecular electronic structure, magnetism, spectroscopy, and reactivity of transition metal complexes. The participants will have the opportunity to obtain knowledge and develop skills in the use of theory and computational chemistry to understand and predict spectroscopic properties of open-shell systems, enriching their view on how modern electronic structure methods are employed in transition metal research.

Lecturers

- Frank Neese
- Serena DeBeer
- Alexander Schnegg
- Eckhard Bill
- Frank Wennmohs
- Thorsten Glaser
- Dimitrios A. Pantazis
- Maurice van Gastel
- Shengfa Ye
- Thomas Weyhermüller

Topics

- Introduction to computational chemistry
- Ligand field theory and optical spectroscopy
- X-ray spectroscopy and Crystallography
- Nuclear magnetic resonance spectroscopy
- Electron paramagnetic resonance spectroscopy
- Magnetic Circular Dichroism Spectroscopy
- The ORCA program system
- Magnetochemistry
- Mössbauer spectroscopy
- Reactivity
- Vibrational spectroscopy

A series of Special Interest Lecture will also be offered on advanced topics of experimental techniques and computational methods.

Organizers:

Dimitrios A. Pantazis, Serena DeBeer, Frank Neese

<http://www.cec.mpg.de/workshops/summerschool2019>



This Summer School is part of the International
Max Planck Research School on Reactive Structure
Analysis for Chemical Reactions (IMPRS-RECHARGE).

