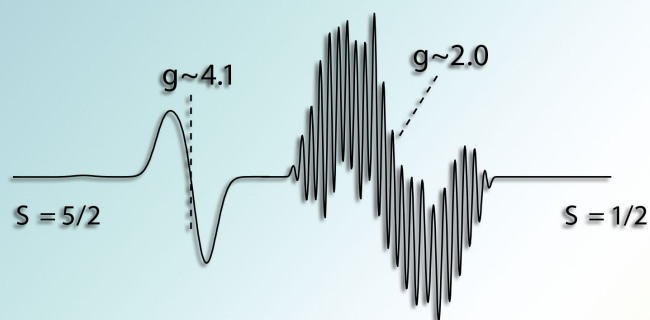


Summer School 2014

Methods in Molecular Energy Research: Theory and Spectroscopy

August 31 - September 6, 2014

Wissenschaftspark Gelsenkirchen, Germany



$$A_{iso}^{(K)} = \pm A_{iso,BS}^{(K)} \left(\frac{\langle S_z \rangle_{BS}}{S_A} \right) \left(\frac{\langle S_z^{(A)} \rangle}{S_f} \right)$$

This summer school is designed for graduate students and post-doctoral fellows in the general field of inorganic chemistry and molecular energy research. Participants will be introduced to a wide range of spectroscopic methods by international experts, while practical sessions will focus on calculations of electronic structure and spectroscopic properties with quantum chemical methods.

Topics

- Basic density functional theory calculations
- Ligand field theory, Spin Hamiltonian formalism
- EPR, X-ray spectroscopies (XAS/XES), Mössbauer, MCD, Vibrational spectroscopy (FTIR/Raman)
- Calculation of spectroscopic parameters
- Advanced special interest lectures

Lecturers:

- Franc Meyer
- Felix Tuczek
- Thorsten Glaser
- Eckhard Bill
- Frank Neese
- Maurice van Gestel
- Serena DeBeer

Organizers: Maurice van Gestel, Dimitrios Pantazis, Eckhard Bill
MAX PLANCK INSTITUTE FOR CHEMICAL ENERGY CONVERSION

More information and registration:
<http://www.cec.mpg.de/workshops/summerschool2014>