CFEL SCIENCE

SEMINAR

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Building 99, Seminar Room I+II (EG)

Christoph R. Jacob

Institute of Physical and Theoretical Chemistry, TU Braunschweig

Theoretical Spectroscopy of Complex Chemical Systems

Quantum-chemical calculations are essential for the assignment and interpretation of spectra of small molecules as well as complex molecular systems. Large molecular systems present a significant challenge not only because of the increasing computational effort that is required for an accurate quantum-chemical description, but also require new approaches for the interpretation of the large amount of data provided by such calculations. On the other hand, small molecular systems with a complicated electronic structure, such as transition metal complexes, pose additional challenges and their theoretical spectroscopy also requires novel quantum-chemical approaches.

In my talk, I will outline some of our work concerning the theoretical spectroscopy of such complex chemical systems, focussing on the vibrational spectroscopy of biomolecules and on the X-ray spectroscopy of transition metal catalysts.

For vibrational spectroscopy, I will discuss how switching from the commonly used normal modes to localized modes can aid the interpretation of harmonic vibrational spectra [1] and how such localized modes can provide significant benefits in the calculation of anharmonic vibrational spectra [2]. For X-ray spectroscopy, I will show how the combination with quantum-chemical calculations can provide insights into the electronic structure of transition metal complexes [3,4] and how it can help reveal the mechanism of the selective catalytic reduction of NO [5,6].

[1] Ch. R. Jacob, M. Reiher, J. Chem. Phys. 130 (2009), 084106.

[2] P. T. Panek, Ch. R. Jacob, ChemPhysChem 15, 3365 (2014).

Host: Melanie Schnell - CFEL Molecular Physics seminar