UNIVERSITÄT LEIPZIG

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Wilhelm-Ostwald-Institut für
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Kolloquium des Wilhelm-Ostwald-Instituts

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Using Ensembles to Evaluate Spectroscopic Properties: Case Studies from Transition Metal Chemistry

Abstract

Quantum chemistry has reached predictive power in the computation of spectroscopic properties for organic molecules, inorganic complexes and materials. Over the past years, the use of ensembles, for instance from molecular dynamics simulations or Wigner sampling, has received increasing attention. The central idea is to generate a representative set of geometric structures at a given temperature, on which single point calculations at a high electronic structure level of theory are performed. Very often, superior results are obtained in comparison to the established approach of predicting the property of interest for a single optimised structure.

In this talk, we will showcase the effect of using ensembles for predicting the infrared spectra of 1,1′-diazidoferrocene, to represent the temperature dependence of quadrupole splitting values obtained from Mössbauer spectroscopy, to discuss charge transfer character in the special pair(s) of Photosystem II, and to analyse the electron transfer paths and their implications for the intervalence charge-transfer band of a mixed-valent ruthenium complex, the Creutz–Taube ion.