Graduate School Seminar

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Molekulare Quantendynamik

Nuclear dynamical correlation effects in X-ray spectroscopy from a time-domain perspective

To date X-ray spectroscopy has become a routine tool that can reveal highly local and element-specific information on the electronic structure of atoms in complex environments.
Despite working on energy scales that are much larger than those corresponding to nuclear motions, taking nuclear dynamics and the associated nuclear correlations into account can be of importance for X-ray spectroscopy. Here, we develop a rigorous time-domain method and establish a reliable and efficient protocol for simulating X-ray spectra from time-correlation functions that explicitly accounts for the underlying nuclear phenomena provided by ground state molecular dynamics simulations. The corresponding results are compared against those from the conventional sampling procedure for gas phase and bulk water. Although the impact of nuclear dynamical effects on the first-order absorption amplitudes is fairly small, second-order resonant inelastic scattering spectra exhibit pronounced fingerprints of nuclear motions. The developed methodology does not depend on the spectral range it is operating on and, therefore, can be applied to, e.g., UV/VIS resonance Raman spectroscopy out-of-the-box.

Talk: English
Slides: English

Location: Institute of Physics, Albert-Einstein-Str. 24, HS1

Talks in SS 2016

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