

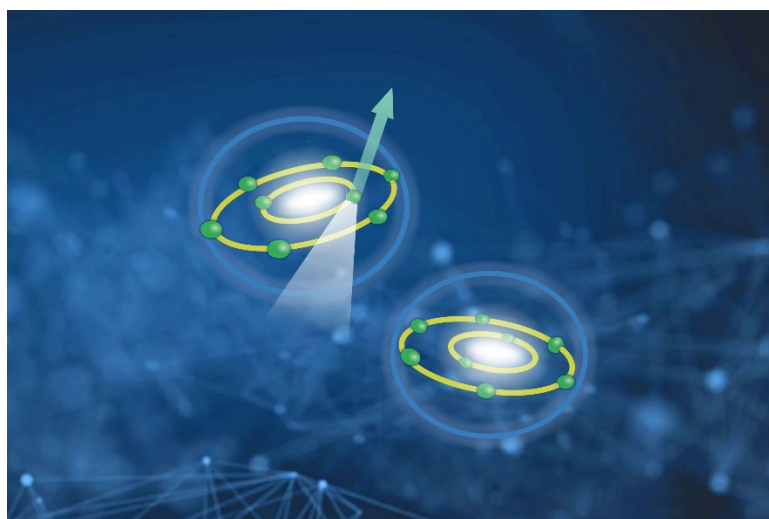
Institutsseminar

Auger Spectroscopies in Liquids: Theoretical Challenges

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Novel X-ray experiments provide a remarkable insight into the electronic structure of liquids and aqueous solutions as well as into the ultrafast processes following ionization. Their potential is thus enormous, they can provide evidence on mechanisms of X-ray impact on molecules or provide spectroscopic signatures of different chemical environments. The experiments, however, require a complex theoretical interpretation that must also include accurate solvent models and their coupling to developing approaches for core-excited or ionized molecules. In my talk, I will focus mainly on approaches for local and non-local Auger processes (such as normal Auger decay, Intermolecular Coulombic Decay (ICD) or Electron Transfer Mediated Decay (ETMD) following X-ray impact and I will describe models that we use for modelling complex environments. The models include fragmentation approaches (QM:QM), polarizable continuum models or explicit polarizable force fields within the QM:MM scheme. With the developed theoretical toolkit we attempt to interpret the experimental Auger-type spectra and explore the effects of X-ray radiation in liquids.



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