セミナーのお知らせ

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Advances in the theory of X-ray absorption spectroscopy for the study of novel nanomaterials

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Abstract:

X-ray absorption spectroscopy (XAS) is a powerful tool for probing the atomic and electronic structure locally around atoms of a selected element. While the general theory of XAS is well understood, it is necessary to make the computational methods more accurate and predictive, especially for the analysis of complex nanoscale materials. In this seminar I present recent advances in the theory and computation of XAS spectra and show applications to oxide nanoparticles and metal organic molecules. First, the electronic structure of titania nanoparticles is studied using O K-edge XAS and density functional theory. By analyzing the linear dichroism, the crystallographic orientation of individual nanoparticles can be deduced. Next I introduce multichannel multiple scattering theory which includes particle-hole multiplet coupling in an ab initio manner. The theory is applied to L23-edge spectra of light 3d-elements and reveals the subtle interplay between intra-atomic electron correlation, ligand field and band structure effects. Finally, L23-edge XAS and X-ray magnetic circular dichroism are calculated using an improved ligand field multiplet model, where all model parameters are obtained from density functional theory. XAS spectra of adsorbed organic molecules with transition metal centers (phthalocyanines and porphyrins) are analyzed and the complex spin and orbital ground state of these molecules is determined.

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