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Determination of the local structure in metal-complexes by combining XAS and XES

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Nanoscale local atomic structure determines most of unique properties of novel materials without long range order. To study its fine details one has to use both computer nanodesign and advanced experimental methods for nanodiagnostics. The status of modern theoretical analysis of the experimental x-ray absorption spectra to extract structural parameters is presented. Novel in-situ technique for nanodiagnostics - extracting of 3D structure parameters on the basis of advanced quantitative analysis of X-ray absorption near edge structure (XANES) - has been developed. The possibility to extract information on bond angles and bond-lengths (with accuracy up to 0.002 nm) is demonstrated and it opens new perspectives of quantitative XANES analysis as a 3D local structure probe for any type of materials without long range order in atoms positions (all nanostructured materials and free clusters belong to this class of materials). Even more possibilities are opening by using simultaneously several experimental synchrotron based techniques: XANES and XES and/or RIXS. In the framework of these approaches, the results of recent studies of local atomic structure for several types of nanostructures including nanoclusters with different types of chemical bonding, core-shell nanoneedles and thin films of dilute magnetic semiconductors, 5d-transition metal-organic complexes, Cu1+ and Cu2+ binding sites in amyloid-β peptide, Co aqua complexes in aqueous solution, nanostructured materials for hydrogen storage and nanocatalysts based on zeolites and MOF are reported. Along with the calculations of conventional XANES and XES, we show a possibility to simulate core-to-core and valence-to-core RIXS as well. Molecular orbitals (or DOS) of metal complexes can be directly related to the peaks in XES spectra in RIXS maps. This information is essential for understanding of electronic structure of metal complexes and design of novel materials.

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