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Multi-scale molecular dynamics & first-principle calculations of X-ray absorption spectra: the coordination of metal cations with water e biomolecules.

Wednesday, 11 December 2019 15:30 (15 minutes)

The progress in high performance computing we are witnessing today offers the possibility of accurate ab initio calculations of structures of systems in realistic physico-chemical conditions. In this talk we present a parameter-free strategy aimed at performing a first-principle computation of the low energy part of the X-ray Absorption Spectroscopy (XAS) spectrum, based on density functional theory (DFT).
The starting model system configurations are built by means of classical molecular dynamics simulations calculations of metal-water complexes. Then, DFT is exploited to relax the resulting metal-water geometrical structures. Finally the XAS spectra associated to the resulting structures are calculated.
As first applications we determined the coordination mode of divalent metal cations in water, showing that Cu(II) and Zn(II) ions have different coordination modes. Here we will show preliminary results obtained in the more interesting - and much more computationally expensive - case in which metal ions are in complex with molecules of biological relevance, such as the amyloid beta peptides involved in the pathogenesis of Alzheimer's disease.

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