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Multi-scale molecular dynamics & first-principle calculations of X-ray absorption spectra: an application to the study of metal cation coordination in water

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The progress in high performance computing we are witnessing today offers the possibility of accurate ab initio calculations 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).
As a first application we apply this strategy to determine the coordination mode of Cu(II) and Zn(II) in water. The necessary model system configurations are built starting from classical molecular dynamics (MD) and tight-binding calculations on 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. The comparison with experimental data shows that the Zn(II) spectral features are nicely reproduced from structures with an octahedral Zn(II) coordination, while the Cu(II) spectrum can be properly reproduced assuming a weighted combination of penta- and hexa-coordinated Cu(II).
The success of the approach in these two paradigmatic cases makes us optimistic about the possibility of extending our strategy to the calculation of XAS spectra of Cu(II) and Zn(II) ions in the more interesting - and much more computationally demanding - case in which they are in complex with molecules of biological relevance, such as, for example, the amyloid beta peptide involved in the pathogenesis of Alzheimer's disease.

Primary authors: DE SANTIS, Emiliano (ROMA2); STELLATO, Francesco (ROMA2); ROSSI, Giancarlo (ROMA2); LA PENNA, Giovanni (R); MORANTE, Silvia (ROMA2); MINICOZZI, Velia (ROMA2)

Presenter: STELLATO, Francesco (ROMA2)

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