Réunions scientifiques

Séminaires

Séminaire SOLEIL

Coupling X-ray Absorption Spectroscopy and Molecular Dynamics Simulations to Solve Structures of Solutions Containing Heavy Metal Ions.

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Grand Amphi SOLEIL

Structural and dynamic properties of metal ions in aqueous solution have long been a classical topic in solution chemistry due to their huge number of applications in chemistry, physics, biology, earth sciences, and engineering. The determination of their solvation and/or coordination structure in solution is a key-point in understanding the physicochemical properties, as well as their migration and diffusive behaviour through solid porous phases, condensed systems and inter-phases.[1]

Among the reduced number of experimental techniques which can supply information on the ion environment, X-ray Absorption Spectroscopy (XAS) have gained importance during the last decades.[2] However, the XAS data analysis is not free of difficulties as the high correlation among factors affecting the amplitude, the large number of multiple scattering paths which may contribute to the global signal and the need of a model structure to be taken as reference.[3] During the last fifteen years implementations of methods for the absorption phenomena based on the inclusion of independent information derived from quantum mechanics and computer simulations for both EXAFS and XANES spectra have been incorporated to reduce the degree of uncertainty in the analysis of the XAS spectra.[4]

This presentation describes the ensemble of quantum and statistical methods employed to simulate XAS spectra and the type of synergy derived from the combination of the theoretical and experimental information.[5] A set of cases studied by computer simulations (Monte Carlo and Molecular Dynamics) where aqueous solutions of several trivalent d-transition metal cations, such as Cr^{3+}, Rh^{3+} and Ir^{3+},[5b,6] and transuranide, Cf^{3+},[7a] as well as an antitumoral Pt(II)-complex is presented.[7b]

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