Réunions scientifiques

Séminaires

Séminaire SOLEIL

Ultrafast X-ray absorption study of solvation dynamics and EXAFS study of ion-pair structure in aqueous solution

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Invité par François BAUDELET

Lundi 17 mars à 14h30
Grand Amphi SOLEIL

Solvation dymamics is the change of the solvent shell structure around a solute upon electronic changes of the solute. It is therefore at the core of condensed phase chemistry and of biology. Here we use a novel approach that allows a direct visualization of the structural changes of the solvent shell in real-time. It uses iodide in water and combines ultrafast optical and X-ray spectroscopies in a pump-probe scheme. A femtosecond laser pulse excites the solute impulsively, while another optical pulse and/or an X-ray pulse, whose time delay can be tuned with respect to the first pump pulse, will take snapshots of the changes that result from excitation. Pico and femtosecond X-ray absorption near edge structure (XANES) spectra were recorded from 300 fs up to several nanoseconds. They were analyzed with respect to the different photoproducts observed on these time scales, delivering spectra for the intermediate reaction products, I0 and I-2. Analysis of transient EXAFS at 50 ps delivers a solvent shell expansion of ~0.6 Å with respect to that of ground state iodide. Femtosecond transient XANES spectra show an increase in the binding energies of the 5*p* and 2*s* electron, with respect to those at 50 ps. This indicates different solvent structures and thus the transition from hydrophilic to hydrophobic occurring over 4 ps during which a transient I-OH2 species is formed.

In this seminar I also discuss our study of ion hydration structure and ion-pair structure in aqueous halide salts. Depending on ions type, its concentration and solution condition, different ion structures and ion associations are formed. We developed methods for studying structure of simple ions in aqueous solution using a combination of EXAFS, XRD and molecular dynamics (MD) simulation. Hydration structure of ions Ca2+, Cl-, Rb+, Br- were successfully derived using X-ray absorption/diffraction simultaneous refinement (XADSR), a new method that simultaneously refines EXAFS and XRD data. The accuracy of the structure is benefited from the complimentary of EXAFS and XRD techniques.

I also present some of our operando XAFS studies of catalyst structure of heterogeneous Pd nanoparticles for reaction of benzene and phenol hydrogenations in a variety of different liquid phase solvents including water, toluene, iso-propanol at 200°C and 50 bar. We found clear chemical state and structural change of Pd nanoparticles.

Ce séminaire sera suivi d'une pause-café

Formalités d'entrée : accès libre dans l'amphi du Pavillon d'Accueil. Si la manifestation a lieu dans le Grand Amphi SOLEIL du Bâtiment Central, merci de vous munir d'une pièce d'identité (à échanger à l'accueil contre un badge d'accès).

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