Institut de Minéralogie et de Physique des Milieux Condensés
Unité Mixte de Recherche 7590
B77, 4 Place Jussieu F-75252 Paris CEDEX 05

SÉMINAIRE
Vendredi 11 février, 14h30

Salle de Conférence, 4ème étage, Tour 22-23, Salle 1
IMPMC, Université P. et M. Curie, 4, Place Jussieu, 75005 Paris

HIDEKAZU IKENO

Fukui Institute for Fundamental Chemistry, Kyoto University

INTRODUCTION OF *AB-INITIO* MULTIPLET METHOD FOR X-RAY ABSORPTION SPECTROSCOPY

The metal $L_{2,3}$ x-ray absorption spectra (XAS) of 3*d* transition metal (TM) compounds shows widely spread multiplet structures because of the strong interaction between the core TM-2*p* and 3*d* electrons. The development of *ab-initio* method to simulate TM-$L_{2,3}$ XAS is an issue with great interest.

In this talk, the *ab-initio* multiplet method for TM-$L_{2,3}$ XAS is introduced. This method is equivalent to the configuration interaction method in quantum chemistry using small cluster models. All ligand field effects can be taken into account by using molecular spinors instead of atomic spinors. Charge transfer from ligands to TM atoms can also be included. Experimental spectra from many compounds with different 3*d*-electron numbers and coordination numbers have been successfully reproduced without any empirical parameters. The effects of the ligand field and charge transfer on spectral shapes will be discussed.

Tel**: 33-(0)1 44 27 42 20** --Fax**: 33-(0)1 44 27 44 69** -
Courriel**:catherine.dreyfus@impmc.jussieu.fr**