Contribution ID : **88** Type : **Presentation**

X-ray absorption Near Edge spectroscopy applied to the study of local atomic structure of ions in solution, e.g., Arsenic.

Thursday, 13 August 2015 09:30 (0:30)

Abstract content

We performed x-ray absorption spectroscopy measurements on the Arsenic K-edge of As(III) in solution under acidic conditions. X-ray near edge structure (XANES) spectra were compared with theoretical calculations which use local atomic structure configurations, derived from either density functional theory (DFT) energy minimization (EM) calculations, or based on classical Monte Carlo (MC) simulations, for a As(OH)3 cluster surrounded by water molecules. Calculations of XANES using either DFT-EM or the average configuration obtained from MC simulations do not reproduce the XANES spectra in the vicinity of the absorption edge. However, specific local atomic structural configurations of the As(OH)3 and water molecules, obtained from MC simulations, which show ordering of water molecules up to 5 Å from the arsenic, reproduce qualitatively the experimental spectra. These results highlight the capability of XANES to yield information about hydration of ions in solution.

Summary

Primary author(s) : Prof. MUSTRE, José (CINVESTAV)

Co-author(s) : Dr. CANCHE-TELLO, Jesús (CINVESTAV); Dr. VARGAS, María Cristina (CINVESTAV); Dr. DEN AUWER, Christophe (Nice Chemistry Institute, Universite Nice-Sofia Antipolis); Dr. ORTEGA BLAKE, Iván (Instituto de Ciencias Físicas, UNAM); Dr. HERNÁNDEZ COBOS, Jorge (Instituto de Ciencias Físicas, UNAM)

Presenter(s) : Prof. MUSTRE, José (CINVESTAV)

Session Classification : Thursday I