

PhD position at IFP-Lyon, in collaboration with ENSCP (2009-2012)

Ab initio simulation of the reactivity of surface acid sites of alumino-silicates

A PhD studentship is available in the field of molecular modelling applied to heterogeneous catalysis, at IFP-Lyon, under the supervision of C. Chizallet (IFP-Lyon), P. Raybaud (IFP-Lyon) and D. Costa (ENSCP). The position is funded by IFP and ANRT for three years, and should start in autumn 2009.

The structure of surface acid sites of amorphous silico-aluminates (ASA) and the origin of their acidity are widely debated in the literature. Understanding the origin of the Lewis and Brønsted acidities of such solids is of first relevance as they are widely used as supports of metallic or sulfide active phases for multifunctional catalysts in fine chemistry, petrochemistry and refining.

Ab initio molecular models of amorphous silicated alumina surfaces have been recently obtained at IFP (C. Chizallet and P. Raybaud, *Angew. Chem. Int. Ed.* 2009 in press). Through a molecular modeling approach, we propose to unravel the link between the structure, the acidity and the reactivity of the new types of acid sites exhibited by ASA surfaces.

This work aims at the calculation of spectroscopic features of the surface sites and reaction pathways for olefin activations. It will allow for detailed comparison with various experimental data such as IR, NMR, XPS and catalytic activity.

Attendees should have strong interests for DFT based calculations applied to catalytic materials and chemical reactivity. For further information or submission of application (CV and motivation letter), please contact:

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