

**PhD position at IFPEN (Lyon - France)
in collaboration with Humboldt University (Berlin - Germany)
(2011-2014)**

***Ab initio* molecular modelling of the impact of de-alumination
and de-silication on the structure and on the acidity of zeolites**

A PhD studentship is available in the field of molecular modelling applied to heterogeneous catalysis, at IFP Energies nouvelles (Lyon, France), under the supervision of C. Chizallet and P. Raybaud, in close collaboration with Prof. J. Sauer (Humboldt University, Berlin, Germany). The position is funded by IFPEN for three years, and should start in autumn 2011.

Solid acids are very important heterogeneous catalysts in the fields of chemistry and refining. In particular, zeolites are microporous crystalline aluminosilicates, exhibiting Brønsted acidity, widely used in industrial plants and studied at the laboratory scale. Their narrow pores may induce diffusion limitations and excessive confinement effects, which leads to the formation of undesired by-products (like over-cracking). The creation of mesopores helps for overcoming these limiting phenomenon. Thus, hierarchical zeolites (micro- and mesoporous) obtained by partial dealumination/desilication of the framework, are the subject of an increasing interest from the scientific community. The mechanisms of the chemical reactions involved by such treatments, and their impacts on the nature of active sites, are still poorly rationalized at the molecular scale. The aim of this PhD work is thus to unravel the formation process, the structure and the behaviour of acid sites by molecular modelling. The simulations will be performed at several scales, to combine the advantages of *ab initio* calculations, necessary for the modelling of the formation and breaking of chemical bonds, that of force-fields calculations, to simulate large systems containing a larger number of atoms. QM/MM and QM/QM methods will also be used for that purpose.

Attendees should have strong interests for density functional theory (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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