Computational Study of Microporous and Mesoporous Molecular Sieves Functionalized with Transition Metal Ions

Professional Summary

The fundamentals of the adsorption and catalysis processes taking place in zeolites functionalized with transition metal ions are still unknown. A clear picture has not emerged on the true presence of transition metals in the framework of molecular sieves. There is also the puzzling experimental observation of cation migration upon adsorption in some of these systems such as those containing Cu, Pd, and Ni. We intend to model these systems using a combination of energy minimizations, molecular dynamics and Monte Carlo methods. As a first step, a full atomic force field has to be validated for these systems. It is also very important to calculate the effective charge present on the metal atom. The system to be study initially is the silicoaluminophosphate SAPO-11 functionalized with Ni, which can be used for catalysis of ethylene dimerization. In this system Ni atoms may be present both as extra-framework cations and as ions incorporated into the silicoaluminophosphate framework. This research will shed light on the role of transition metal ions during catalytic processes taking place in zeolites. It is important to understand whether these ions are mobile during catalysis and if so, whether this mobility is the dominant phenomenon that facilitates catalytic activity.