

BOURSES CHATEAUBRIAND

Proposition de Sujet de Recherche pour l'accueil d'un boursier

Laboratoire

Intitulé du laboratoire

Unité ou numéro (UMR, UPR, etc...) d'identification

Organisme(s) de tutelle

Adresse :

Ville :

Code Postal :

Direction du laboratoire

Nom du Directeur Prénom
Fonction
Téléphone
E-mail

Secrétariat

Téléphone
E-mail
Fax

Thématiques de recherche du laboratoire (en anglais)

Physicochemical properties of materials and devices
Dynamics and reactivity in condensed phases
Environmental Chemistry

Site web du laboratoire :

http://www-lasir.univ-lille1.fr/depart_contact.htm

Proposition de sujet de recherche (en anglais) :

Titre du Projet : First principles study of spontaneous ionization of molecules in nanoporous aluminosilicates

Responsable :

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Description succincte (en anglais) : pour donner *plus de détails*

Already for a long time a group of the laboratory studies the spontaneous ionization and the charge separation phenomena in aromatic molecule/zeolite systems. The reaction runs over different time scales toward a stable radical cation, an electron-hole pair or toward recombination and several factors were found to influence the way in which the reaction occurs (topology of zeolite framework, its composition, nature of charge-compensating cations, size and ionization potential of sorbed molecule). The experimental data obtained already allowed proposing a possible scenario of the processes involved. The project envisages a quantitative theoretical study of the phenomena by means of modern methods of quantum chemistry and it aims at the elucidation of the reaction mechanisms at the atomic level. Thus, at different stages of the project the structure of the molecule-zeolite complex in the initial, intermediate and final states, and the electron solvated in the zeolite framework have to be characterized. An important part of the work is expected can be performed with the use of ab initio molecular dynamics technique. Simplified models based on effective Hamiltonians can also be invoked, if necessary. The challenge of the study arises from the size of the systems of interest and from the fact that an intermediate cation radical state implies the necessity of considering the spin density.

Mots clés (en anglais)

Zeolites

Aromatic
molecules

Spontaneous
ionization

Ab initio
molecular
dynamics

Information(s) complémentaire(s) que vous voudriez communiquer aux candidats intéressés :

The candidate should have a solid background in quantum chemistry and an experience in ab initio molecular dynamics calculations. He will work in a group with a large experience in modeling of nanoporous solids with classical molecular dynamics and in a close interaction with the experimental group working on this topic. All computing facilities will be available at the local, regional or national level.

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