Ab initio molecular dynamics study of bimolecular processes in acid zeolites

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Descrição:

Proyecto asignado a través de la Red Española de Supercomputación (RES [2]).

Many industrially relevant hydrocarbon reactions catalyzed by acid zeolites include in their mechanism bimolecular steps, in which new C-C bonds form by reaction of cationic intermediates with neutral molecules. To design highly specific catalysts able to favor one particular process among some competitive ones, it is necessary to go beyond the static description provided by standard DFT calculations and take into account the mobility of the reactants within the zeolite channels. In this project we intend to investigate, using ab initio molecular dynamics (AIMD) metadynamics simulations, the formation of key dimeric intermediates involved in the diethylbenzene-benzene transalkylation and butene skeletal isomerization reactions, in order to find the zeolite microporous structures able to enhance the rate of such bimolecular steps.

Web:

Ligações

[1] https://itq.upv-csic.es/ [2] https://www.res.es/