Theoretical studies of adsorption on the surface of zeolite ZSM-5

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Keywords: Ab initio calculation, zeolite ZSM-5, Interaction on surface

INTRODUCTION

Chemical reactions involving solid-gas interfaces or solid-liquid are important for varied purposes such as the production of non-renewable resources, materials processing, enhancement of modern technologies, energy production, environmental maintenance and natural resources[1]. The potential of these materials is governed by the electronic and structural characteristics of bulk and their surfaces and the interaction with these molecules adsorbed on them. Understanding the process, describe the reaction mechanisms occurring on their surfaces and get control of products can provide important insights for understanding and development of new devices[2]. In the early 1970s, researchers at Mobil synthesized zeolite ZSM-5 (Zeolite Socony Mobil) and found their catalytic properties in hydrocarbon synthesis[3]. Electronic and structural properties of solids, as the interaction of their surfaces with adsorbent molecules studied can be by electronic structure calculations.

METHODS

Theoretical calculations and relaxation geometries with DFT (Density Functional Theory) method with B3LYP (Becke, three-parameter, Lee-Yang-Parr) 6-31G* based function, PM6 (Parametric Method 6) and MM (Molecular Mechanic) using ONIOM (Our own N-layered Integrated Molecular Orbital and Molecular Mechanics) combining PM6/DFT, PM6/MM, MM/DFT on ZSM-5 zeolite models with 288 atoms (Figure 1-a). A specific pore diameter (Figure 1-b) was chose to be the interactions of molecules of ethanol and calculating the interaction energy in the adsorption process.

RESULTS AND DISCUSSION

The geometry models of ZSM-5 can modify distance values and bond angles between atoms at the end of the convergence calculations. The relaxation of the whole molecule ZSM-5 is not feasible due to the large number of atoms, thereby starting the method using ONIOM treatment of the system with semi-empirical method or molecular mechanics and the other with DFT can be good results. The interaction of ethanol molecules in optimized designs then provide the information on the catalytic reactivity of aluminumsilicate as adsorption energies, bond distances among others.

a) b)

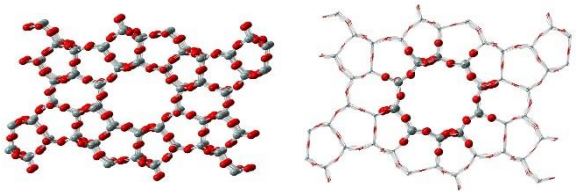

Figure 1. Zeolite ZSM-5 model (a) and specific Pore of adsorption (b).

CONCLUSIONS

Theoretical calculation ab initio of optimization using ONIOM facilitate convergence due to partial treatment of the system. The ethanol interactions in a specific pore of the ZSM-5 model can used to identify and represent the active site of the molecule via data such as bond distances and energies.

ACKNOWLEDGMENTS

The authors are grateful for the support given from the FAPDF, CAPES, CNPQ.

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