Supawadee Namuangruk 2007: Molecular Design of Nanostructured Catalysts for Industrial Reactions. Doctor of Philosophy (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Professor Jumras Limtrakul, Ph.D. 143 pages.


The nanostructured catalysts, which are faujasite and ZSM-5 zeolites, have been modeled by the ONIOM method to investigate the reaction mechanisms of the chemical reactions. Faujasite zeolite is modeled by the 84T cluster and represented by the ONIOM3(MP2/6-311++G**:HF/6-31G*:UFF) methods. This model gives accurate adsorption energies between the adsorbates and the zeolite. The computed adsorption energies are −8.73, −13.91, and −20.11 kcal/mol, which compared well with experimental values of −9.0, −14.0, and −20.4 kcal/mol for ethylene, benzene, and ethylbenzene, respectively. Whereas, ZSM-5 zeolite is modeled by using the 46T cluster and treated with ONIOM2(B3LYP/6-31G**:UFF) method. Both ONIOM models are then used to explore the reaction mechanisms of the alkylation of benzene with ethylene, the dimerization of ethylene, and the isomerization of propene oxide to carbonyl compounds. The obtained information is important for being a basic knowledge in the design of new and better catalysts for the interested reactions.


In addition, the possibility of using carbon nanotube, high surface area and high mechanical strength nano-material, as the catalyst for conversion of toxic nitrous oxide ($N_2O$) to non-toxic nitrogen molecule is also studied. By using quantum cluster approach at B3LYP/6-31G* level of theory, the reaction mechanisms of nitrous oxide decomposition over sidewall of carbon nanotube are investigated. The results show that the Stone-Wales defect site appears to have high catalytic activity over perfect one.

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