Winyoo Sangthong 2009: Structures & Reactions of nanoporous and nanostructured Materials: In silico Nanoscale Design. Doctor of Philosophy (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Professor Jumras Limtrakul, Ph.D. 98 pages.

Density functional theory (DFT) at B3LYP/6-31G(d,p) level of theory and the our-Own-N-layered-Integrated molecular Orbital + molecular Mechanics (ONIOM) at well carlibrated ONIOM(B3LYP/6-31G(d,p):UFF) have been employed to investigate the structures of formaldehyde in Na-exchanged faujasite zeolite and their complexed with propylene. The reaction takes place in a concerted reaction step. The inclusion of the zeolite framework has an influence on the structure and energetics of the adsorption complexes and leads to a lower energy barrier of the reaction (25.1 kcal/mol) as compared to the bare model system (34.4 kcal/mol). If the naked Na ion interacts with the isolated complex, the energy barrier of the system is even lower than the zeolitic system (17.5 kcal/mol), due to the large electrostatic field.

Molecular dynamics simulations of *n*-hexane in siliceous MCM-41 materials, revealed a result of confinement, the adsorption energy of hexane increases when the pore sizes decrease. Also, the adsorption energy increases when the loading is increased from one *n*-hexane molecule to the saturation limit. The self-diffusion coefficients decrease with increasing loadings and when the pore sizes decrease. For low loadings the *n*-hexane molecules lie parallel to the pore channel for every pore size. When the loading is increased, they build up concentric rings.

The stability of nanoclusters and nanocluster-based polymorphs of a range of alkali halides (MX; M= Li, Na, K, Rb, Cs and X= F, Cl, Br, I) are investigated using plane wave density functional theory calculations. For the $(MX)_{12}$ clusters, the slab cluster isomers are found to be the most stable cluster type except, for the lithium halide series (LiX). The energy difference between the rock salt phase (rs-MX) and the sodalite phase (SOD-MX) is found to follow the same trend as that between the respective slab and cage $(MX)_{12}$ clusters. Correspondingly, the lithium halide sodalite phases (SOD-LiX) are all found to be metastable energetically with respect to the lithium halide rock salt forms (rs-LiX).

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