

339. Density Functional Investigation of the Dissociative Adsorption of Benzene on Si(100) Surface

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Density functional total-energy methods are employed to study the C-H bond cleavage process of benzene and polyaromatic species adsorbed on Si(100) surfaces. Past studies show that there are two possible configurations for Benzene adsorbing on a single silicon cluster dimer. This work is extended using larger silicon dimer models to include the cleavage products and the decomposition mechanism. The result shows a triplet configuration of the adsorbed product has to be introduced in order to describe the C-H bond cleavage for both adsorption configurations. Currently, we are investigating the singlet-triplet crossing point geometry and crossing probability. Once completed, the reaction mechanism from the free molecule/cluster to the final cleavage products, together with the transition states and intermediates, can be obtained.