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ADORPTION STRUCTURES OF BENZENE ON A SI(5 5 12)-2X1 SURFACE: A COMBINED STM AND THEORETICAL STUDY

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In a first ever attempt to study the adsorption of organic molecule's adsorption on a high-index Si surfaces, we examined investigated the adsorption of benzene on Si(5 5 12)-(2x1) by using variable-low temperature scanning tunneling microscopy (STM) and density functional theory (DFT) calculations. Several distinct adsorption structures of the benzene molecule were revealed for the benzene molecule. In one structure, The benzene molecule binds with to two adatoms between the dimers of *D3* and *D2* unit cells as in a tilted butterfly type configuration. This structure is produced by the formation of di-σ bonds with the substrate and of two C=C double bonds in the benzene molecule. In another structure, a the molecule adsorbs on honeycomb chains, which have a low adsorption energy because of higher strain effects. Our DFT calculations predicted that the adsorption energy of benzene to be 1.03~1.20 eV on the adatoms and 0.22 eV on the honeycomb chains.