

Chemisorption of Toluene on Si(100): an ab-initio study.

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Adsorption of small organic molecules on the Si(100) surface is a topic of great recent interest since it represents the first stage of technologically relevant processes such as the growth of the Silicon Carbide and CVD diamond film on the silicon surface. Interestingly, a recent STM study suggests that adsorption of toluene occurs only on top of the dimer rows, giving rise to several binding geometries that closely resemble those of benzene. It has also been found that, increasing the temperature, the C leaves the surface, leading to the formation of small SiC cluster. We performed ab-initio Car-Parrinello simulations (geometry optimisation and molecular dynamics) with a slab geometry: DFT (LSD approximations and PBE gradient-correction used) with norm-conserving pseudopotentials and Γ -point sampling of the Brillouin Zone. Complementary calculations have been done using classical MD simulations based on a semiempirical potential (Extended Brenner potential). Two different supercells have been used for modelling the silicon surface at different coverages and for investigating finite-size effects. We have studied adsorption of toluene on Si(100) considering both dissociated and undissociated configurations, by calculating electronic and conformational structure of the stable configurations. Favourable reaction paths have been investigated with the corresponding energy barriers leading from one stable adsorption structure to another one by using the “nudged elastic band method”. Simulations of thermal desorption processes, aimed at describing the early stages of SiC growth, are still in progress.