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Energetics of benzene and phenol adsorption on a TiO_2(110) surface S. DAG, J. ZHOU, S. KALININ, S. OVERBURY, D. MULLINS, A. BADDORF, V. MEUNIER, Oak Ridge National Laboratory — Using large-scale density functional theory calculations, we have studied the structural and electronic properties of benzene and phenol adsorbed on a TiO_2 (110) surface. We found that at low coverage, a benzene molecule impinging to the TiO_2 surface is most likely to be adsorbed flat on the surface 3.3 Å above the Ti row, such that the $C_{2'}$ symmetry axis of the molecule is oriented along the top Ti row, between consecutive bridging oxygen rows. Because of the high repulsive energy between benzene and bridging oxygens, benzene molecules diffuse in quasi one-dimensional channels along a Ti row. At high coverage, benzene molecules organize in a chain-like fashion with two of their C-C bonds being oriented alternatively parallel and perpendicular to a Ti row. The interaction of phenol molecules on the same surface has also been studied. In this case, the adsorption is much stronger and involves interaction between multiple phenol molecules and bridging oxygen rows. Results of our calculations are in excellent agreement with experimental STM data.

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