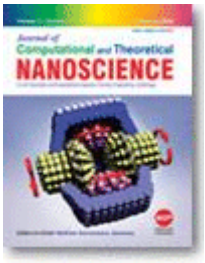

Sulfur Radicals as Tethers for the Adsorption of Aromatic Molecules on Silicon Surface

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Abstract | References | Citations | Supplementary Data | Suggestions

In this work we employ the state of the art pseudopotential method, within a generalized gradient approximation to the density functional theory, to investigate the adsorption process of benzenethiol and diphenyl disulfide with the silicon (001) surface. A direct comparison of different adsorption structures with Fourier transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS) allow us to identify that benzenethiol and diphenyl disulfide dissociatively adsorb on the silicon surface. In addition, theoretically obtained data suggests that the C_6H_5 SH:Si(001) presents a higher Schottky barrier height contact when compared to other similar aromatic molecules.

Keywords: CHEMISORPTION; DENSITY FUNCTIONAL THEORY; ORGANIC MOLECULES; SILICON; SURFACE ELECTRONIC PHENOMENA

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