

A DFT study of adsorption of copper-dioxolene complex at a gold surface

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A problem of a modification of the electronic and magnetic structure of a metalorganic complex by the process of chemisorption at a metallic surface is studied.[1] A model of a Cu-dioxolene complex is proposed and analyzed with the help of the density functional theory (DFT). Various conformations of both neutral and positively charged model complex are considered.[2] Next the molecule is connected to the Au(111) surface with alkanethiol linkers. A study of the dependence of the electronic and spatial structure on the linker length is performed. The conclusion is that properties of molecule are well preserved during the adsorption process and that the charge transfer from the molecule to the metallic substrate is slightly affected by the length of the linking chain.

References:

[1] J. V. Barth, *Surface Sci.* **603**, 1533 (2009).

[2] P. Verma, J. Weir, L. Mirica, and T. D. P. Stack, *Inorg. Chem.* **50**, 9816 (2011).

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