Abstract Submitted
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The electronic and structural properties of the self-assembled monolayer of Au-benzene-1,4-dithiol-Au molecules[1] T.-H. LU, Y.-H. TANG, M.-H. TSAI, Department of Physics, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan — The electronic and structural properties of the self-assembled monolayer of Au-benzene-1,4-dithiol-Au molecules are calculated by first-principles calculation methods. The Au-S bond length obtained is 2.20Å, which is about 6.8% smaller than the sum of their covalent radii of 2.36 Å. The Au-S-C bond angle obtained is 98.9^0, which is within the range of known bond angles of S, e.g. $\angle$FSF=98.2^0 forSF_2, $\angle$ClSCl =$103^0$for SCl_2 and $\angle$CSH =$96.4^0$for CH_3CH_5-SH. The Au 5d band is dominantly located at -2.3 eV below the Fermi level, E_F, with a sharp peak in the partial density of states (PDOS). The PDOS's also show that the highest-occupied-molecular-orbital band contains S 3p, C 2p and Au 5d hybridized states, while the lowest-unoccupied-molecular-orbital band contains S 3p, C 2p, Au 6s and Au 5d hybridized states. The dominant Au 6s states are located at about -1.5eV and 1.3eV relative to E_F. The present result shows that Au 5d states, which are usually ignored in previous theoretical studies, play an important role in the S-Au bonding and contribute significantly to the transport property of the molecule.

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