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Adsorption and conductance of BDT on the Au(111) surface A. FAZZIO, RENATO B. PONTES, FREDERICO D. NOVAES, ANTONIO J.R. DA SILVA, Instituto de Fisica - Universidade de Sao Paulo — Molecular electronics is a new trend in the science and technology at the nanometer-scale. A prototypical system where transport properties have been widely studied both experimentally and theoretically is benzene-1,4-dithiolate (BDT) on Au(111). We present, using Total Energy Density Functional Theory calculations, a detailed study of such a system for different surface coverages and sites, and we find that except at high enough coverages, the BDT lowest energy configuration has the molecule almost lying down on the Au surface. We also find that when the BDT is bridging two Au(111) leads, this lying down configuration still has the lowest energy when compared to the standing up configuration (by approximately 0.4 eV). We have also calculated, using a DFT-based non-equilibrium Green's Function formalism, the conductance for a variety of BDT configurations, including how they vary as a function of the separation between the leads. We find that due to resonant features in the conductance, it can vary significantly depending on the distance between the leads. We also calculate the total energy, forces and conductance for a variety of BDT configurations for different separation between leads. We thank the Brazilian agencies FAPESP and CNPq, and CENAPAD-SP for computer time.

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