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Ferrocenyl-alkanethiolate on the Au(111) surface: Electronic and transport properties in density functional theory SHUCHUN WANG, WENCHANG LU, JERRY BERNHOLC, Department of Physics, North Carolina State University, Raleigh, NC 27695-8202 — Self-assembled monolayers of organic molecules on the gold surface have shown a number of interesting features, such as non-linear conductance and negative differential resistance (NDR). We focus here on ferrocenyl-alkanethiolate on the Au(111) surface, for which NDR has been observed in experiments. In order to understand conduction through the ferrocenyl-alkanethiolate, we investigate its atomic and electronic structure on the surface, as well as its electron transport properties within density functional theory. The real-space multigrid method and ultrasoft pseudopotentials are used to examine various surface configurations with different molecular coverages. We find that the attachment of ferrocenyl significantly reduces the packing density of alkanethiolates on the gold surface. The saturation coverages for different molecular species will be discussed. The conductances and I-V curves, calculated using non-equilibrium Green's functions expanded in variationally optimized localized orbitals, are analyzed in terms of resonant tunneling and modification of molecular levels under bias.

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