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First-principles investigation of electronic coupling effects between organic molecules and transition metal electrodes on conduction GUNN KIM, MARCO BUONGIORNO NARDELLI, J. BERNHOLC, North Carolina State University, Raleigh — We investigate electronic transport in long chain molecules sandwiched between metallic electrodes. The calculations are carried out using the non-equilibrium Green function method and a basis set of localized orbitals, which are optimized to minimize the DFT total energy of the system. The optimization is performed on a grid, using multigrid techniques to accelerate convergence. Our model systems consist of saturated hydrocarbon (alkane) chains having thiol (-SH) and amino (-NO_2) end groups attached to transition metal electrodes. We show that the current-voltage characteristics strongly depend on the coupling between the molecule and the metal electrodes.

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