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Ab-Initio calculations of electron transport properties of Si-Porphyrin-Si devices FILIPE J. RIBEIRO, WENCHANG LU, JERRY BERNHOLC, North Carolina State University, Raleigh NC 27695-7518 — We present results of numerical calculations of the electronic transport properties of devices consisting of porphyrin molecules connected to Si(100) leads. Our calculations are based on ab-initio ultrasoft pseudopotentials and the generalized gradient approximation (GGA) to the exchange and correlation energy functional. Transport properties were calculated using a non-equilibrium Green's function method in a basis of optimally localized orbitals. We studied three different molecules: H2-, Zn-, and Ni-porphyrins. The somewhat different alignments of the HOMO and LUMO levels of the molecules with the top of the valence and bottom of the conduction bands of the Si leads has strong implications on the I-V characteristics of the devices. In particular, the turn-on voltages are different for the different molecules. In addition, if the Si leads are heavily doped n-type, regions of negative differential resistance exist in all three systems.

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