

Abstract Submitted
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Effect of doping and molecular coverage on the I-V characteristics of organic molecules on silicon surfaces WENCHANG LU, N.C. State University, V. MEUNIER, ORNL, S. WANG, Q. ZHAO, J. BERNHOLC, N.C. State University — Quantum transport properties of organic molecules on the silicon (001) surface have been studied by ab initio non-equilibrium Green function calculations in a basis of optimal localized orbitals. Our calculated results provide a qualitative picture and quantitative understanding of the importance of self-consistent screening and broadening of quasi-molecular orbitals under a large bias. Negative Differential Resistance (NDR) is found to be a general feature of organic molecules on Si surfaces [1]. By comparing the I-V characteristics of a monolayer of cyclopentene molecules with that of a single molecule, we show that interactions between the molecules attenuate the NDR, as seen in experiments. We have also investigated the effects of proximal dopant atoms on the NDR in a large unit cell.

[1]. W. Lu, V. Meunier, J. Bernholc, Phys. Rev. Lett. 95, 206805 (2005).

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