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Non-equilibrium quantum transport properties of organic molecules on silicon WENCHANG LU, North Carolina State University, Raleigh, V. MEUNIER, ORNL, Oak Ridge, J. BERNHOLC, North Carolina State University, Raleigh and ORNL, Oak Ridge — Electronic and quantum transport properties of organic molecules on Si surfaces are studied within density functional theory. This system is synthetically accessible and has potential applications in chemical sensors, resonant tunneling devices and molecular logic. Since the bonding of organic molecules on Si is well defined and often well characterized, it constitutes an ideal model system for systematic comparisons with experiment. The 1,4-diethynylbenzene molecule on Si(111) was chosen as a first example. A non-equilibrium Green's function approach with an optimized localized orbital basis is employed to investigate transport properties under different biases. Due to variational optimization, only a small number of basis functions per atom are needed, enabling studies of systems containing up to 1000 atoms. For each system, the interface structure is optimized by massively parallel total energy calculations. The I-V curves show a number interesting features, including a plateau and a negative differential resistance. The origins of these features and applications to other systems will be discussed.

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