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Theoretical study of electron transport through π-stacked ethylbenzene lines bonded to a Si surface MANUEL SMEU, Center for the Physics of Materials and Department of Physics, McGill University, Montreal, QC, Canada, ROBERT WOLKOW, National Institute for Nanotechnology and Deparment of Physics, University of Alberta, Edmonton, AB, Canada, HONG GUO, Center for the Physics of Materials and Department of Physics, McGill University, Montreal, QC, Canada — Recently, experimental techniques were developed for lines of π-stacked ethylbenzene molecules to self-assemble on an H-terminated Si (100) surface in the laboratory of one of the authors. In this work, we use density functional theory (DFT) combined with the nonequilibrium Green's function formalism (NEGF) to model electron transport through these ethylbenzene lines to determine if they could be used as molecular wires. In our calculations, the molecules are bonded to an H-terminated Si (100) surface and are bridging two Al leads. The transmission spectrum and its associated scattering states are determined by the NEGF-DFT technique. The presence of the Si substrate is found to play an important role for conduction: there is a dominant transmission peak near the Fermi level which is contributed by the Si substrate and not the π-stacked molecular line. The low-bias resistance is found to increase exponentially with the length of the molecular line, indicating a tunneling behavior in conduction.

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