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Calculation of Single-Electron Transport Through Molecules
JINGBIN LI, NIKITA SIMONIAN, KONSTANTIN LIKHAREV, Department of Physics and Astronomy, Stony Brook University — We have carried out numerical calculations of electron transport through OPE terminated with isocyanide groups. The electron spectra and orbitals are calculated using the NRLMOL DFT package (http://cst-www.nrl.navy.mil/∼nrlmol/). The wave functions are then used to calculate the transmission of the interface energy barriers, within the Bardeen approximation. If the transmission is high, we calculate the current using the standard methods of the theory of ballistic field effect transistors, while if it is sufficiently low, we use the general theory of single-electron tunneling in systems with discrete energy spectrum [1]. (In order to understand the best way of resolving the problems due to the intrinsic limitations of the DFT approach, initial calculations have been carried out for a simple model: a Na atom sandwiched between two Au electrodes.) Our results yield I-V curves with substantial negative differential resistance (NDR) of conducting branches, due to a new mechanism: the enhancement of one of the tunnel barriers of the system by the applied electric field. The work is supported in part by AFOSR and NSF. [1]. D. V. Averin, A. N. Korotkov, and K. K. Likharev, Phys. Rev. B, 44, 6199 (1991).

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