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Universal Negative Differential Resistance in Single-Electron Transport through Atoms and Molecules NIKITA SIMONIAN, JINGBIN LI, KONSTANTIN LIKHAREV, Department of Physics and Astronomy, Stony Brook University — We have carried out numerical calculations of single-electron transport through single atoms and organic molecules (OPE chains terminated with isocyanide groups), weakly coupled to gold electrodes. The calculations were based on the general theory of single-electron tunneling in systems with discrete energy spectrum [1], with molecular orbitals obtained by the ab initio DFT solver NRLMOL [2]. The Kohn-Sham potential calculated by the solver was also used to calculate the wavefunctions of "external" electrons, so that the necessary overlap integrals could be obtained using the Bardeen formula [3] rather from the NEGF approach. The most remarkable result of the calculations is the virtually unversal negative differential resistance, due to a new physical mechanism resulting from the suppression of transparency of one of the tunnel barriers of the system by the applied source-drain 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). [2] See http://cst-www.nrl.navy.mil/∼nrlmol/. [3] J. Bardeen, Phys. Rev. Lett. 6, 57 (1961).

Nikita Simonian
Department of Physics and Astronomy, Stony Brook University

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