Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Negative Differential Resistance at Low Bias: C60-Based Molecular Devices WENCHANG LU, North Carolina State University, Raleigh, NC and CSMD, ORNL, TN, XIAOHONG ZHENG, NC State University, Raleigh, NC, T.A. ABTEW, NC State University, VINCENT MEUNIER, CSMD, ORNL, TN, JERRY BERNHOLC, NC State University, Raleigh, nC and CSMD, ORNL, TN — Unlike single-C60-based devices, molecular assemblies based on two or more C60 can exhibit negative differential resistance (NDR). We evaluate electron transport properties of molecular devices built from two C60 connected by an alkane chain, using a non-equilibrium Green function technique implemented within the framework of linear-scaling DFT. We find that electronic conduction in these systems is mediated by C60's lowest unoccupied molecular orbitals (LUMOs), as in the case of a single-C60-based device. However, as the LUMOs' positions are pinned to the chemical potentials of their respective electrodes, their relative alignment shifts with applied bias and leads to an NDR at a very low bias. Furthermore, the position and magnitude of the NDR can be tuned by chemical modification of the C60s and by changing the length of the alkane linker. The flexibility and richness of C60-based molecular electronics components point to a potentially promising route for the design of molecular devices and chemical sensors.

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Date submitted: 30 Nov 2010 Electronic form version 1.4