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C_{60}-based devices: large scale simulations and design X. H. ZHENG, W. LU, T. A. ABTEW, NC State University, V. MEUNIER, Oak Ridge National Laboratory, J. BERNHOLC, NC State University — C_{60} is one of the most promising building blocks in the design of molecular devices, due to its spherical symmetry and structural reproducibility. In this work, the electron transport properties of two- and three-terminal devices built of C_{60}s are investigated. The C_{60}s are connected by alkane chains and then sandwiched between aluminum nanowires. The calculations are carried out using a massively parallel real-space multigrid O(N) implementation of density functional theory. The conductance and nonlinear I-V characteristics are evaluated by a nonequilibrium Green function method in a basis of optimally localized orbitals (W. Lu, V. Meunier, and J. Bernholc, PRL 2005). A conduction mechanism mediated by the LUMOs of the C_{60} molecules is revealed. Due to the bias effect on the LUMO alignment, negative differential resistance (NDR) is observed in both two- and three-terminal devices at a very low bias. Since the LUMOs can be easily modified by molecular adsorption, the NDR position is tunable and can be used in sensor applications without the need for specific molecular receptors.

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