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Spin-polarized electron transport in a molecular wire: tuning the conductivity through conformational changes L. SENAPATI, S.C. ERWIN, Center for Computational Materials Science, Naval Research Lab, Washington DC, R. PATI, Department of Physics, Michigan Technological University, Houghton MI
— We investigate theoretically the electrical conductivity of a molecular wire consisting of three linked benzene molecules. By using magnetic electrodes the conductivity becomes spin-dependent, the degree of this dependence varying with the relative spin-alignment of the two electrodes. Of particular interest is how the the conductivity depends on the geometrical conformation of the benzene wire. Here we use density-functional theory and the Landauer-Büttiker method to calculate this dependence from first principles. We find that the current depends sensitively on the conformation, with a near-planar configuration of the three benzene rings giving significantly higher current (by $\sim$30%) than the ground-state non-planar structure.

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