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Prediction of Ultra-High ON/OFF Ratio Nanoelectromechanical Switching from Covalently Bound C_{60} Chains

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Applying a first-principles computational approach combining density-functional theory and matrix Green's function calculations, we have studied the effects [2+2] cycloaddition olligormerization of fullerene C_{60} chains on their junction charge transport properties. Analyzing first the microscopic mechanism of the switching realized in recent scanning tunneling microscope (STM) experiments, we found that, in agreement with experimental conclusions, the device characteristics are not significantly affected by the changes in electronic structure of C_{60} chains. It is further predicted that the switching characteristics will sensitively depend on the STM tip metal species and the associated energy level bending direction in the C_{60}-STM tip vacuum gap. Considering infinite C_{60} chains, however, we confirm that unbound C_{60} chains with strong orbital hybridizations and band formation should in principle induce a much higher conductance state. We demonstrate that a nanoelectromechanical approach in which the C_{60}-STM tip distance is maintained at short distances can achieve a metal-independent and drastically improved switching performance based on the intrinsically better electronic connectivity in the bound C_{60} chains.

Keywords: Oligomerized fullerenes, Molecular switches, First-principles simulation, Scanning tunneling microscopy