A Novel Prospective of Molecular Electronics: Electric Field-Controlled Switch, Diode, and Spin-Filter

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ABSTRACT

In this work, we suggest a novel single molecular diode with switching and spin-filtering prospective based on an endohedral fullerene, where the triplet-state of a titanium atom, encapsulated inside a C_{70} fullerene cage, controls switching, rectification, and spin filtering of the species. In order to investigate the switching behavior of the system, we applied external electric fields via two and four electrodes such that the orientation of the enclosed atom inside the cage can be controlled by the orientation of the electric field. Hence, the implemented electrodes can assist the electron transportation through the system in addition to switching the single atom using the applied voltages. Results demonstrate that the applied voltage can significantly decrease the energy barrier between two identical local minima by stabilizing the transition state of the switching process. Besides, density functional theory merged with non-equilibrium Green's function have been employed to explore spin-filtering and conductivity aspects of the model system. Our results suggest that this system exhibits a significant spin-filtering property as well as a negative differential resistance at low bias voltages. The exceptional properties of the studied system, switching via oriented external electric field and the conductivity with spin-filtering prospective, suggest the potential of this single molecule system in nano-electronics and nano-spintronics applications.

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