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**Spin-dependent Transport through a Magnetic Carbon-Nanotube-Based Molecular Junction**[1] CHUN ZHANG, LINLIN WANG, HAI-PING CHENG, Physics Department, University of Florida, XIAOGUANG ZHANG, Oak Ridge National Lab, YONGQIANG XUE, State University of New York — We apply a first-principles computational approach to study the transport properties of a magnetic molecular junction, which consists of two Fe-doped carbon nanotubes (CNT) (6, 0) and a $C_{60}$ molecule in the linear response regime. The conventional local spin-density functional theory (LSDFT) approach is applied to study the band structure of Fe-doped CNT. We find that for majority spin, only one band crosses the Fermi level while for minority spin, four bands cross the Fermi level. A method that combines LSDFT and non-equilibrium Green's functions technique is used to study the CNT/C60/CNT junction. For situations in which the net magnetic moments of two CNTs are parallel, we find that the conductance of minority-spin electrons is two times higher than the conductance of majority-spin electrons, which is rarely seen for the spin-dependent tunneling through layered structures. The magnetoresistance (MR) ratio is found to be 11%. Our calculations suggest that CNTs have great potential in spintronics.

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