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Spin-polarized transport through the endohedral fullerene $Gd@C_{82}$ LAXMIDHAR SENAPATI, STEVEN C. ERWIN, Center for Computational Materials Science, Naval Research Laboratory, Washington, DC 20375 — We investigate theoretically the spin-polarized electron transport through an endohedral metallofullerene $Gd@C_{82}$ sandwiched between magnetic Fe contacts. Using density-functional theory and the Landauer-Buttiker formalism, we demonstrate that the total current depends on the relative orientation of the Gd spin and the two Fe-contact spins. Specifically, the current varies by 15-20% as the orientation of the Gd spin moment is changed with respect to that of Fe contacts. We also studied the effect of changing the strength of the coupling between the Fe contacts and the fullerene molecule. We find that strong coupling leads to metallic current-voltage characteristics, while weak coupling leads to Coulomb blockade.

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