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Simulation of electron conduction in a prototypical three-terminal molecular transistor HAIYING HE, RAVINDRA PANDEY, Department of Physics and Multi-Scale Technology Institute, Michigan Technological University, Houghton, MI 49931, SHASHI KARNA, US Army Research Laboratory, Weapons and Materials Research Directorate, ATTN: AMSRD-ARL-WM; Aberdeen Proving Ground, MD 21005-5069 — In a single molecule, electronic charge can be modulated either by electrical field or by chemical effects, thereby opening up the possibility of their use as active elements in electronic devices. In this talk, we present the results of a theoretical study on the electronic conduction of a novel, three-terminal molecular architecture, analogous to a heterojunction bipolar transistor. In this architecture, two diode arms consisting of donor-acceptor molecular wires fuse through a ring, while a gate modulating wire is a π-conjugated wire. The calculated results show the enhancement or depletion mode of a transistor by applying a gate field along the positive or negative direction. A small gate field is required to switch on the current in the proposed architecture. The changes in the electronic conduction can be attributed to the intrinsic dipolar molecular architecture in terms of the evolution of molecular wavefunctions, specifically the one associated with the terphenyl group of the modulating wire in the presence of the gate field.

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