Theory of Molecular Transistor

Haying He,[a] Ravi Pandey,[a] and Shashi P. Karna[b]
[a]Michigan Technological University, Department of Physics and Astronomy, 1400 Townsend Drive, Houghton, MI 49931 USA
[b]US Army Research Laboratory, Weapons & Materials Research Directorate, ATTN: AMSRD-ARL-WM, Aberdeen Proving Ground, MD 1005-5069 USA

Organic molecules with controllable electron transport offer themselves as a potential candidate for future nano-molecular electronics. Due to such potential applications, there has been intense interest in developing a fundamental understanding of electron transport in molecular systems. To date, much of these studies have been focused on understanding the physics and chemistry of electron transport under external electric bias across a molecule in two-terminal architecture. Two-terminal architectures offer applications such as interconnect, diodes, and rectifiers. In order to extend the application space of organic molecules in electronics, we have performed *ab initio* density theory calculations of a three-terminal molecular architecture with a goal to develop a fundamental understanding of field-modulated molecular transistors. The two-arms of the molecule consisting of *np-pn* type heterojunction architecture and built from organic aromatic backbones substituted with acceptor and donor functional groups acts as e*mitter* and *collector*, respectively.. The third-arm consisting of an aromatic terphenyl molecule acts as *base*. Our calculation suggests that a field applied along the "base" moiety easily modulates the current across emitter and collector. The calculations further reveal that the direction of the external electric field at the base moiety is more important than its magnitude in modulating current across the emitter and collector arms. In this paper, we shall present the results of our calculations and discuss in details the effects of different parameters, including the magnitude and directions of the field, metal-molecule junctions, and polarizability of the donor-acceptor substituted molecular architecture, on the switching properties of the molecule. .