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Switching of Current in a Molecular Junction[1] KAMAL DHUNGANA, SUBHASISH MANDAL, RANJIT PATI, Michigan Technological University — Achieving atomic level control at the metal-molecule interface in a single molecule conductance measurement is a difficult task that hinders the progress in molecular electronics. The lack of atomic level structural information of the interface makes the theoretical interpretation of experimental data much harder. Herein, we create an ensemble of device structure by varying metal-molecule binding sites, the orientation of the molecule at the interface, interface distance, and conformational change within the molecule to study junction dependent conductance behavior in Ruthenium-Bis(terpyridine) molecular wire, which has been fabricated and characterized. An orbital dependent DFT in conjunction with a parameter free, single particle Green's function approach is used to study the I-V characteristics. Our calculation for the weakly-coupled ONTOP junction geometry yields a relatively small (OFF state) current value below a threshold voltage (V_{th}). The current value is found to increase at V_{th} and remains flat (ON state) after the threshold value. A similar non-linear I-V curve with a current switching behavior has been reported experimentally.

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