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A Single Diblock Molecular Diode TOBECHUKWU JOSHUA OBODO, ALTYNBEK MURAT, UDO SCHWINGENSCHLÖGL, PSE Division, KAUST, Saudi Arabia — We investigate the rectification behavior of the diblock dipyrimidinyldiphenyl molecule and its derivates with increasing donor groups using self-interaction corrected density functional theory combined with the non-equilibrium Green's function method. In particular, we study a tandem setup for the representative optimized rectifier, finding that it significantly improves the rectification behavior of the molecular diode. Moreover, we find that the molecule consisting of donor and acceptor mimics a pn-junction, whereas the tandem setup does not behave as a pn-pn junction, rather like a p-np-n junction. Our results help explain the mechanism behind the experimentally observed rectification behavior of the molecule.

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