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First Principles Study and Theoretical Analysis of a Single Molecular Diode by $p-n$ di-block molecules HISAO NAKAMURA, YOSHIHIRO ASAI, National Institute of Advanced Industrial Science and Technology, JOSH HIHATH, NONGJIAN TAO, Arizona State University — The concept of a single molecular diode was first proposed by Aviram and Ratner, and there have been many studies of synthesis D-σ-A or $p-n$ di-block molecules and measurements of the current-voltage ($I-V$) characteristics for relating molecular junctions. Recently, the $I-V$ measurement in a symmetric tetraphenyl junction and non-symmetric dipyrimidinyl -diphenyl diblock junction was performed, and clear rectification was found in the latter system, which resembles the $p-n$ junction by the covalent connection between electron-deficient bypyrimidinyl and electron-rich biphenyl moieties, though an applied bias is much lower than the resonant level. In this presentation, we performed the first principles calculations of electron transport for the above tetraphenyl and dipyrimidinyl -diphenyl diblock junctions by the self-consistent nonequilibrium Green's function theory with the use of our HiRUNE program module. We carried out the systematic analysis of the rectification behavior and identified the change of electron-pathway in the bridge molecule relating to $p-n$ junction based on the first principles data. The relation between the rectifying action and molecular conformation, particularly, the torsion of diblock, will be discussed.

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