Electron correlation enhancement of the diode property of asymmetric molecule

YOSHIHIRO ASAI, HISAO NAKAMURA, National Institute of Advanced Industrial Science and Technology (AIST), JOSHUA HIHATH, NONGJIAN TAO, Arizona State University — Stimulated by the giant diode property found in tetraphenyldithiol derivative including dipyrimidinil-diphenly diblock [1], a possible mechanism of the giant diode property was investigated theoretically based on electron correlation. We found that the mean field theory (MFT) fails in describing the giant diode property, as it was confirmed by first principle calculation of ballistic electronic current through the diode molecule using GGA. Electron correlation effect on electric current taken into account within the self-consistent GW approximation using Keldysh Green’s function theory was found to give the fair account of the giant diode property. We conclude that elastic electron collision beyond MFT enhances the diode property quite a lot.