

Abstract Submitted  
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**Electron correlation enhancement of the diode property of asymmetric molecule** YOSHIHIRO ASAI, HISAO NAKAMURA, National Institute of Advanced Industrial Science and Technology (AIST), JOSHUA HATH, NONGJIAN TAO, Arizona State University — Stimulated by the giant diode property found in tetraphenylthiol derivative including dipyrimidinil-diphenyl 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.

[1] I.Díez-Pérez et al, Nature Chemistry, 635 (2009).

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