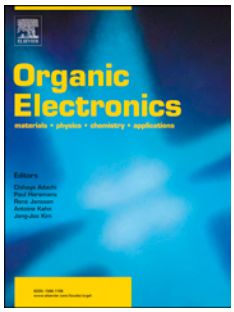
Accepted Manuscript



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PII: S1566-1199(18)30513-5

DOI: 10.1016/j.orgel.2018.09.048

Reference: ORGELE 4914

To appear in: *Organic Electronics*

Received Date: 26 July 2018

Revised Date: 21 September 2018

Accepted Date: 28 September 2018

Please cite this article as: Z.-Q. Wang, Y. Li, X. Niu, M.-Z. Wei, M.-M. Dong, G.-C. Hu, Z.-L. Li, D. Wang, C.-K. Wang, G.-P. Zhang, Controlling the conductance of single-molecule junctions with high spin filtering efficiency by intramolecular proton transfer, *Organic Electronics* (2018), doi: https://doi.org/10.1016/j.orgel.2018.09.048.

Controlling the conductance of single-molecule junctions with high spin filtering efficiency by intramolecular proton transfer

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Abstract

The pursuit of miniaturization of magnetic electronic components spurs intensive theoretical and experimental researches on designing molecule-scale magnetic devices. Controlling the transport properties is one of the most vital focuses for magnetic molecular devices. In this work, magnetic devices constructed by a single epindolidione (Epi) molecule (5,11-dihydrodibenzo[b,g][1,5]naphthyridine-6,12-dione) bridging two zigzag graphene nanoribbon (zGNR) electrodes are theoretically designed. The Epi molecule can be converted between the keto and enol forms, which is confirmed by first principle molecular dynamics method. The influences of intramolecular proton transfer and the bridging manner between the core molecule and zGNR electrodes on the magnetic transport properties are investigated. Spin-resolved current-voltage (I-V) curves show that both the keto and enol devices display remarkable spin filtering effect. However, the effect of intramolecular proton transfer on the electron transport properties depends on the bridging manner between the Epi molecule and zGNR electrodes. When the Epi molecule is connected to zGNR electrodes with 4,7-sites (A bridging manner), the electron transport properties of molecular junctions are hardly affected by the intramolecular proton transfer. On the contrary, the conductance of the molecular junctions is significantly modulated by the intramolecular proton transfer when the Epi molecule is connected to zGNR electrodes with 4,4′-sites (B bridging manner). Further analysis reveals that the high spin filtering effect originates from stronger coupling between spin-up edge electronic states of zGNR electrodes and states of the core molecule. With B bridging manner, the conjugation characteristics of the Epi molecule as well as the transmission pathway of tunneling electrons can be largely modulated by the intramolecular proton transfer. Our work proposes a feasible way to control the conductance of single-molecule junctions by taking advantage of intramolecular proton transfer.

Keywords: Single-molecule junction, Spin filtering effect, Intramolecular proton transfer, Nonequilibrium Green's function method

1. Introduction

As one of the promising approaches to miniaturization of traditional electronic components, designing and synthesizing organic single-molecule devices have been appealing to

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