Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Theoretical Study of the Electron Tunneling through the Spiral Molecule Junctions along Spiral Paths

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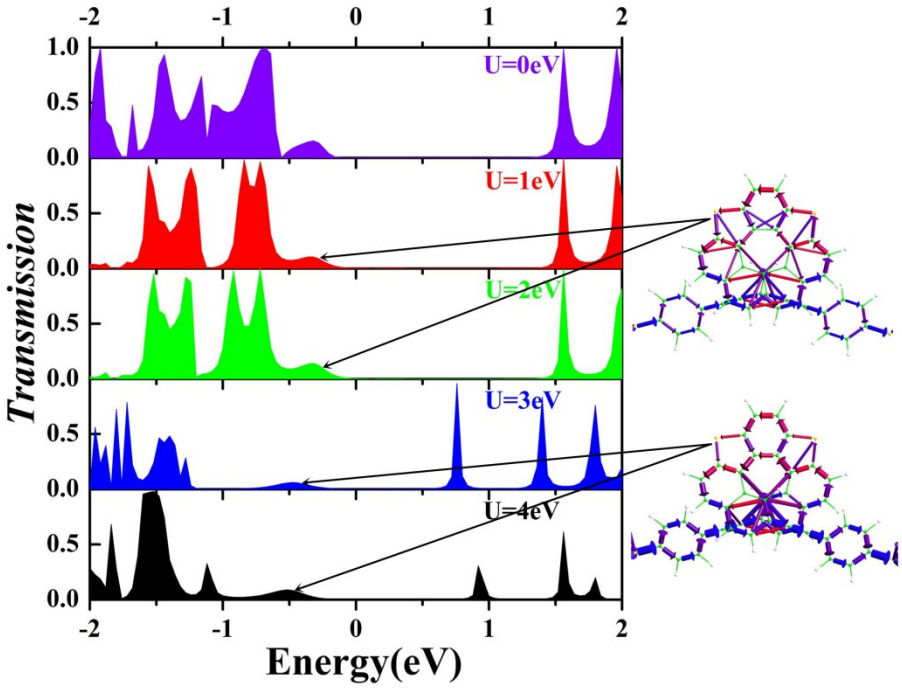

Fig.S1 The transmission spectra of molecular junction S2 changing with the empirical parameterU of sulfur atoms in molecular junction S2

To investigate the effect of the self-interaction corrections, we have calculated the transmission spectra by changing the empirical parameter U of the sulfur atoms of molecular junction S2 taken as an example utilizing GGA+U method, as presented Fig.S1. The U term essentially corrects the self-interaction of electrons in another way in the framework of present KS-DFT scheme(with the present exchange-correlation functionals). With the U changing from 0.0eV to 2.0eV, the self-interaction exert a relatively small effect on the transport resonance peak close to the Fermi level, which contributed by the HOMO and HOMO-1 of the molecule S2. As the U is set to 3.0eV and 4.0eV, the strength of the transmission peak below the Fermi level decreases and the position locates far away from the Fermi level, while the transport resonance peak contributed by the LUMO moves closer to the Fermi level. It indicates that the value of current will become smaller under low bias and have a sharp increase when the LOMO enters the bias window. From analysis above, the transport properties of the molecular junctions is primarily effected by the self-interaction modified approach which can modulate the energy level of spiral molecules effectively. On the other hand, the spiral current at the edges of molecule S2 always

exists and some other tunneling channels are opened with the value of U increasing(shown in Fig.S1). As such effect exists for all those systems investigated and it would be similar among those systems, the variation pattern of the electronic properties would be qualitatively predicted by the PBE method employed.