Supplemental Material for 'Transport property of ligand-driven light-induced spin-change Fe-based spin crossover complexes'

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The proposed molecular junctions include the left (L) and right (R) electrodes, and the extended molecule (C), which contains the sandwiched $Fe(stpy)_4(NCS)_2$ complex, two and three surface layers of the left and right electrodes, respectively. To obtain spin-resolved current through the molecular junction, the transmission coefficients of the molecular junctions are calculated using

$$T_\sigma(E, V) = Tr[\Gamma_L G_\sigma \Gamma_R G_\sigma^+], \quad (1)$$

where σ stands for the spin-up ($\uparrow$) and spin-down ($\downarrow$) channels, $\Gamma_{L/R}$ is the coupling matrix between the extended molecule and the left/right electrode, defined as $\Gamma_{L/R} = i(\Sigma_{L/R} - \Sigma_{L/R}^\dagger)/2$, and G_σ is the spin-dependent retarded Green's function of the extended molecule, calculating by,

$$G_\sigma = [(E + i\eta)S_C - H_C - \Sigma_R - \Sigma_L]^{-1}, \quad (2)$$

here, H_C and S_C stand for the Hamiltonian and overlap matrices of the extended molecule, η stands for a small number, and $\Sigma_L(\Sigma_R)$ is the self-energy due to the presence of the left (right) electrode, which is calculated by

$$\Sigma_{L/R} = V_{L/R} g^{L/R} V_{L/R}^\dagger, \quad (3)$$

where $g^{L/R}$ is the surface Green's function of the left (right) electrode, V_L (V_R) stands for the interaction between the extended molecule and left (right) electrode.

Then the current through the molecular junction is obtained by

$$I(V) = \frac{e}{h} \int T_\sigma(E, V)[f(E - \mu_L) - f(E - \mu_R)]dE, \quad (4)$$

where the f(E-μ) is the Fermi-Dirac function for the left and right electrodes with the chemical potential $\mu_{L(R)}$.

Fig. S1 illustrates the flow chart of the adopted DFT+NEGF method for calculating transport properties in this work.

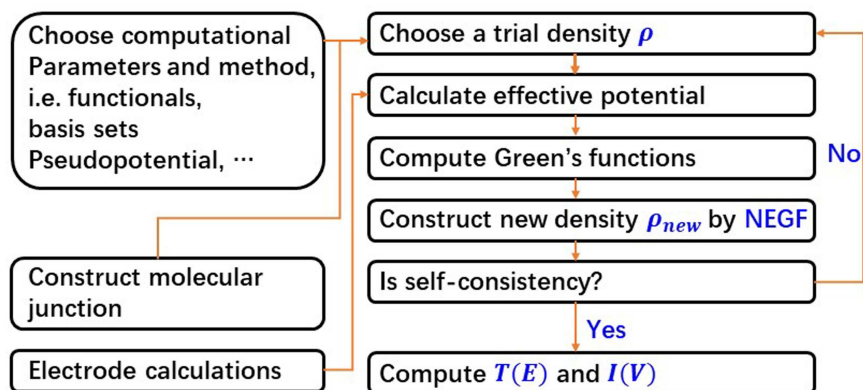* Corresponding author. E-mail: jhuang@ustc.edu.cn
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FIG. 1: Flow chart of DFT+NEGF method.