

Supplementary information

## Electron-doping induced half-metallicity in one-dimensional Co-dithiolene molecular wires

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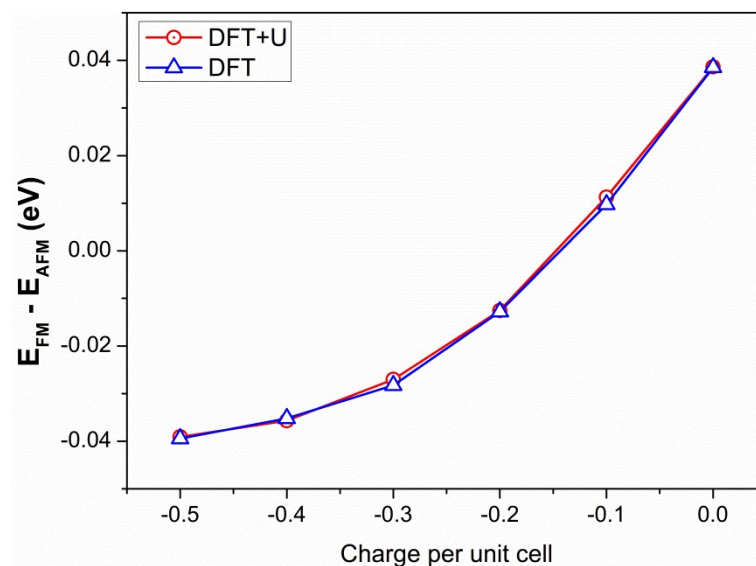


Figure S1. Comparison of the energy difference between FM and AFM ( $E_{FM}-E_{AFM}$ ) *versus* the number of electrons doped into the wire as obtained from DFT+U and DFT calculations, respectively.

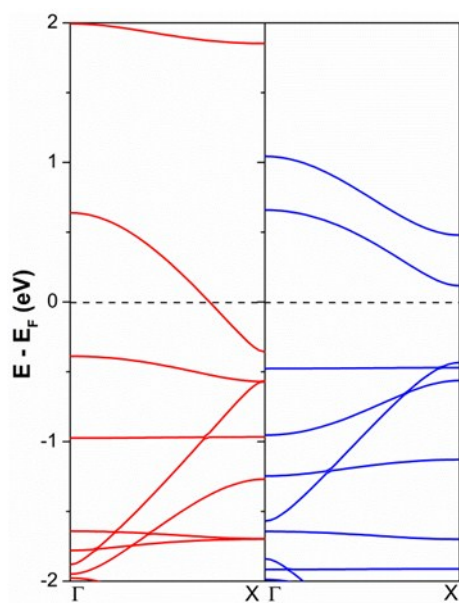


Figure S2. Band structure of electron-doped Co-dithiolene molecular wire with a concentration of 0.3e per unit cell obtained from DFT+U calculations.