## Supporting Information

## Electron transport behavior of quinoidal heteroacene-based junctions: Effective electron-transport pathways and quantum interference

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Figure S1 (a) The molecular structures of  $\alpha$ -S-TC,  $\alpha$ -S-TC-1' and  $\alpha$ -S-TC-2'; (b) the plots of *I-V* curves of these models; (c) the transmission spectra of these molecular junction at zero-bias, where the curves of  $\alpha$ -S-TC-1' and  $\alpha$ -S-TC-2' are the same; and (d) the transmission spectra at 1.0 V bias.