Electronic Supplementary Information

Theoretical Design of a Hole-Transporting Molecule: Hexaaza[1$_6$]parabiphenylophane

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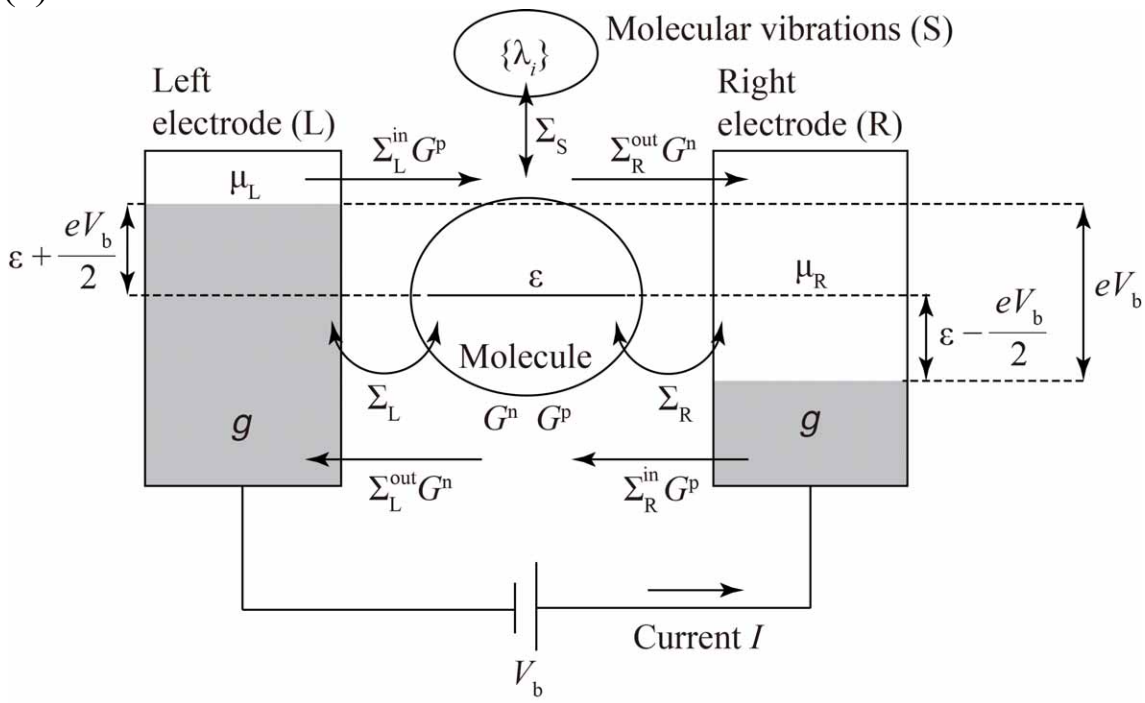
Content:

(a)



(b)

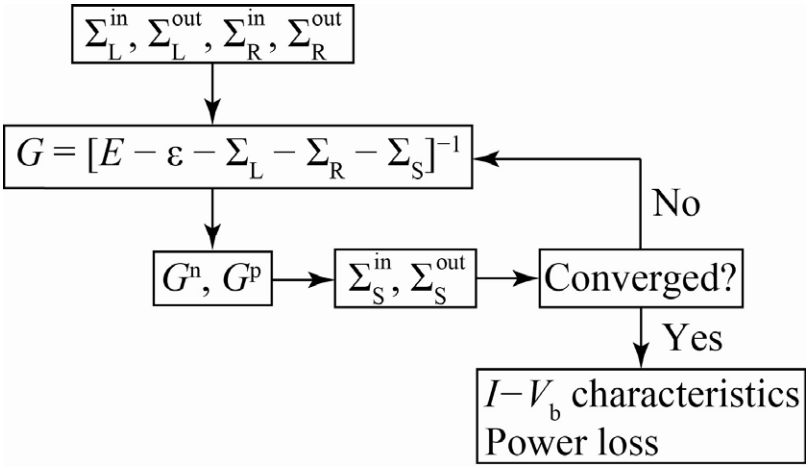


Figure S1. (a) Schematic representation of NEGF method and energy level alignment in this study. (b) Flowchart of a self-consistent calculation of G^{n}, G^{p}, Σ_{S}^{in}, and Σ_{S}^{out}.

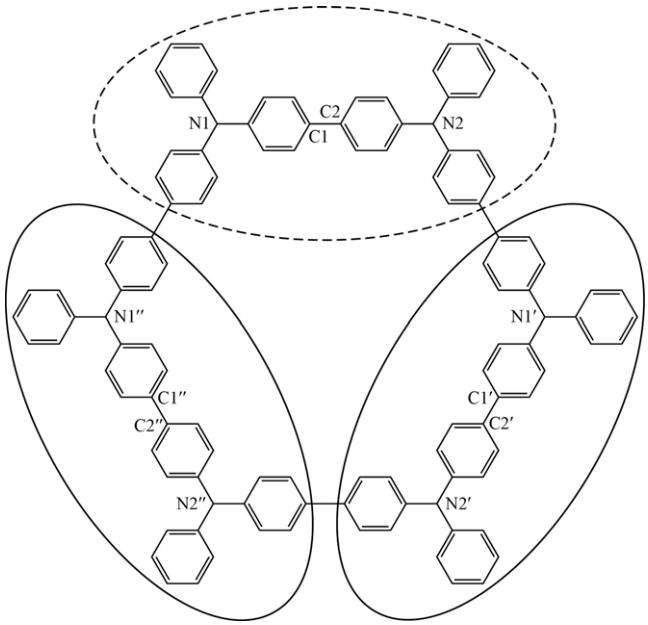


Figure S2. Atomic labeling scheme for HAPBP.

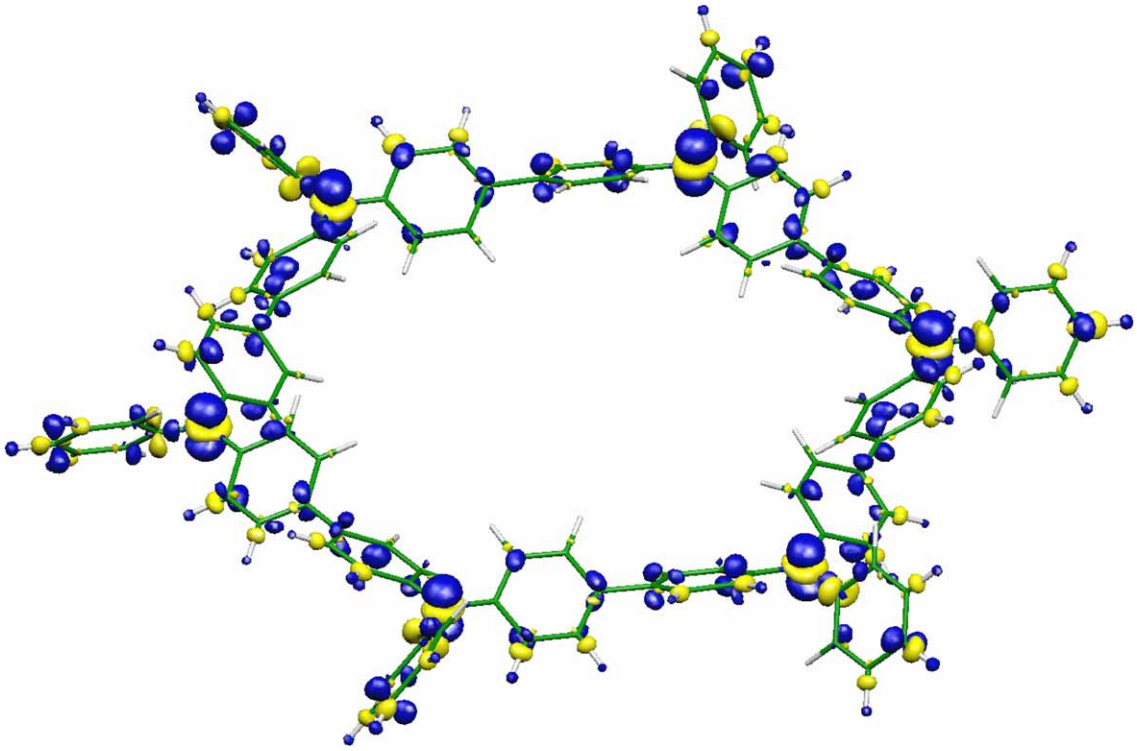


Figure S3. Electron-density difference $\Delta\rho$ for HAPBP with symmetry lowered to C_2 at an isosurface value of 8.0×10^{-4} a.u. Blue shows where values are negative; yellow shows where values are positive.

Table S1. Mulliken charge for nitrogen atoms of neutral HAPBP.

atom	D_6 symmetry	C_2 symmetry
N1	−0.6547	−0.6540
N2	−0.6547	−0.6540
N1′	−0.6547	−0.6545
N2′	−0.6547	−0.6550
N1″	−0.6547	−0.6545
N2″	−0.6547	−0.6550

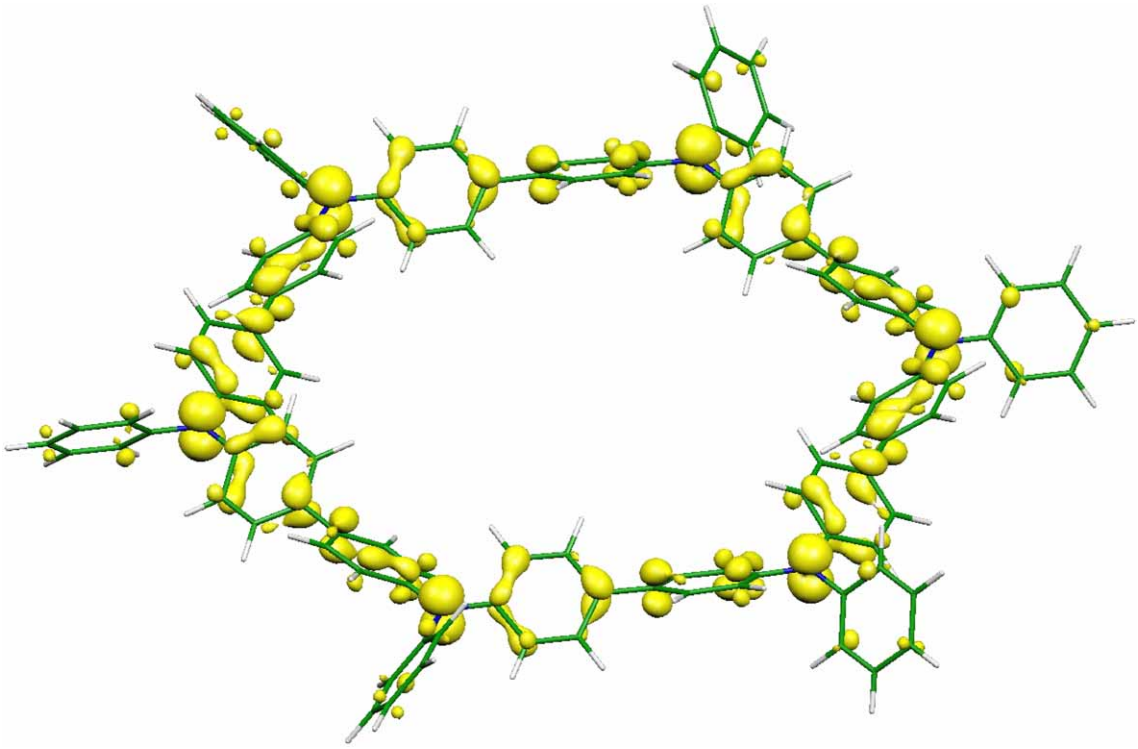


Figure S4. Electron density of HOMO for the neutral HAPBP at an isosurface value of 8.0×10^{-4} a.u.

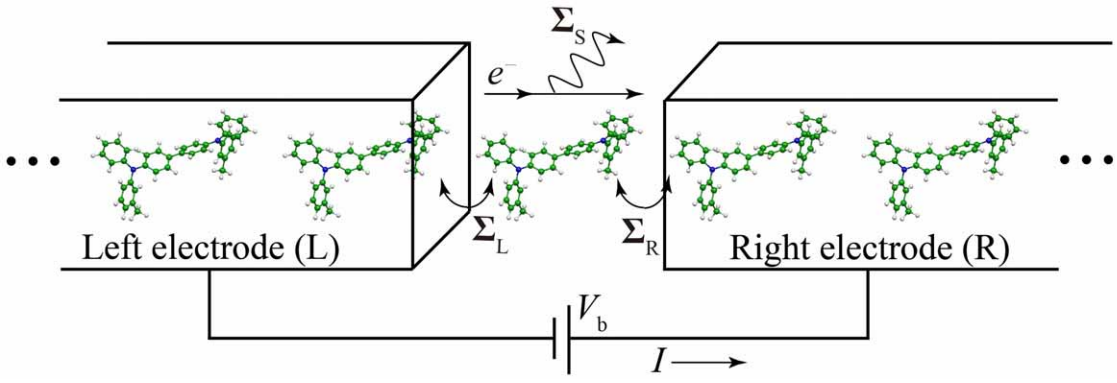


Figure S5. Single molecular conduction between one-dimensional semi-infinite electrodes.