

Electronic Supplementary Information (ESI)

Contents:

1. Computational Method.

We employed density functional theory (DFT) calculations to optimize the geometries of the sensitizer dyes, using the hybrid PBE0 functional⁽¹⁾ and the triple-zeta basis set 6-311G(d,p)⁽²⁾. The Stuttgart effective core potential basis set⁽³⁾ was employed for calculations involving iodine molecule. At the optimized geometries, frequency analyses were performed to confirm that these geometries are true minima on the potential energy surface. All calculations were carried out using the Gaussian09 program package⁽⁴⁾.

2. Cyclic voltammetry curves of dye in CH₂Cl₂ solution.

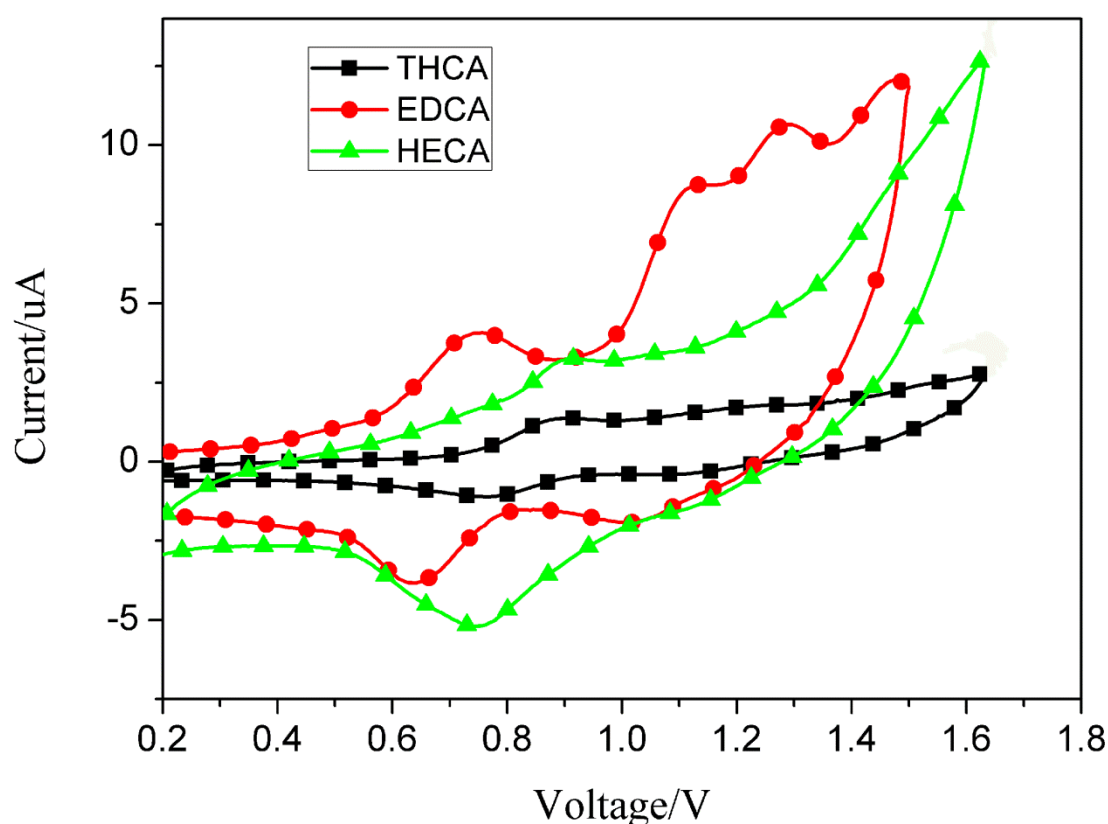
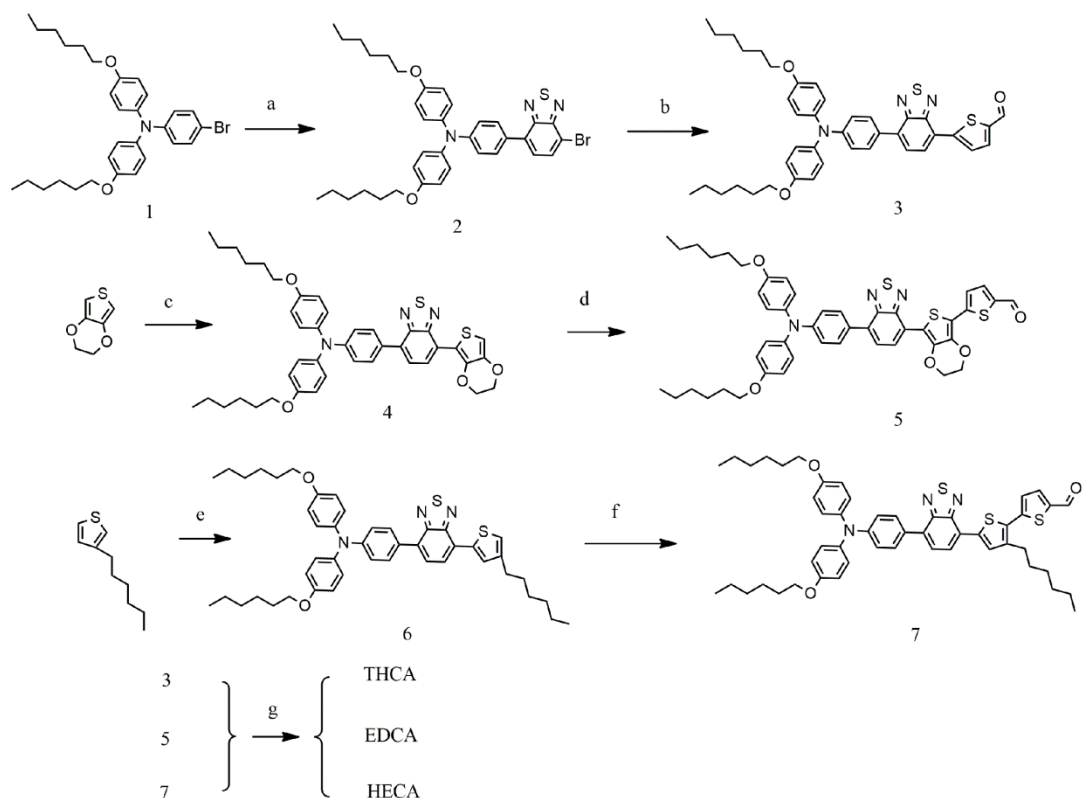


Fig. S1 Cyclic voltammetry curves of dye in CH₂Cl₂ solution.

3. Synthetic routes of dyes.



Reagents and conditions: (a) *n*-BuLi, Isopropyl borate, 4,7-dibromobenzo[*c*][1,2,5]thiadiazole, K_2CO_3 , Pd(dffp)Cl₂, THF, H₂O and N₂ atmosphere. (b) 5-Formyl-2-thiopheneboronic acid, K_2CO_3 , Pd(dffp)Cl₂, THF, H₂O and N₂ atmosphere. (c) *n*-BuLi, *n*-Butyltin Trichloride, Compound 2, Pd(PPh₃)₂Cl₂, toluene and N₂ atmosphere. (d) NBS, CH₂Cl₂ and CH₃COOH, 5-formyl-2-thiopheneboronic acid, Pd(dffp)Cl₂, K_2CO_3 , THF, H₂O and N₂ atmosphere. (e) *n*-BuLi, Isopropyl borate, Compound 2, K_2CO_3 , Pd(dffp)Cl₂, THF, H₂O and N₂ atmosphere. (f) NBS, CH₂Cl₂, 6h, 5-Formyl-2-thiopheneboronic acid, K_2CO_3 , Pd(dffp)Cl₂, THF, H₂O and N₂ atmosphere. (g) acetic acid and ammonium acetate, corresponding aldehyde, cyanoacetic acid.

References

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