

Effect of Heterocyclic and Non-Heterocyclic Units on FDT-Based Hole Transport Materials for Efficient Perovskite Solar Cells: A DFT Study

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Table S1: Energies of HOMO and LUMO for **FDT** obtained in dichloromethane solvent using B3LYP, PBE0, HSE06, and BMK functionals and 6-31Gd,p) basis set. All the energies are in the eV.

FDT	B3LYP	PBE0	HSE06	BMK	Expt. ¹
E_{HOMO}	-4.50	-4.72	-4.35	-5.15	-5.16
E_{LUMO}	-1.80	-2.02	-1.66	-2.45	-2.28

Table S2: Optimal range separation parameters (ω) for all HTMs.

HTMs	FDT	FDT-1	FDT-2	FDT-3	FDT-4	FDT-5	FDT-6	FDT-7
ω	0.006	0.001	0.001	0.001	0.001	0.001	0.001	0.001

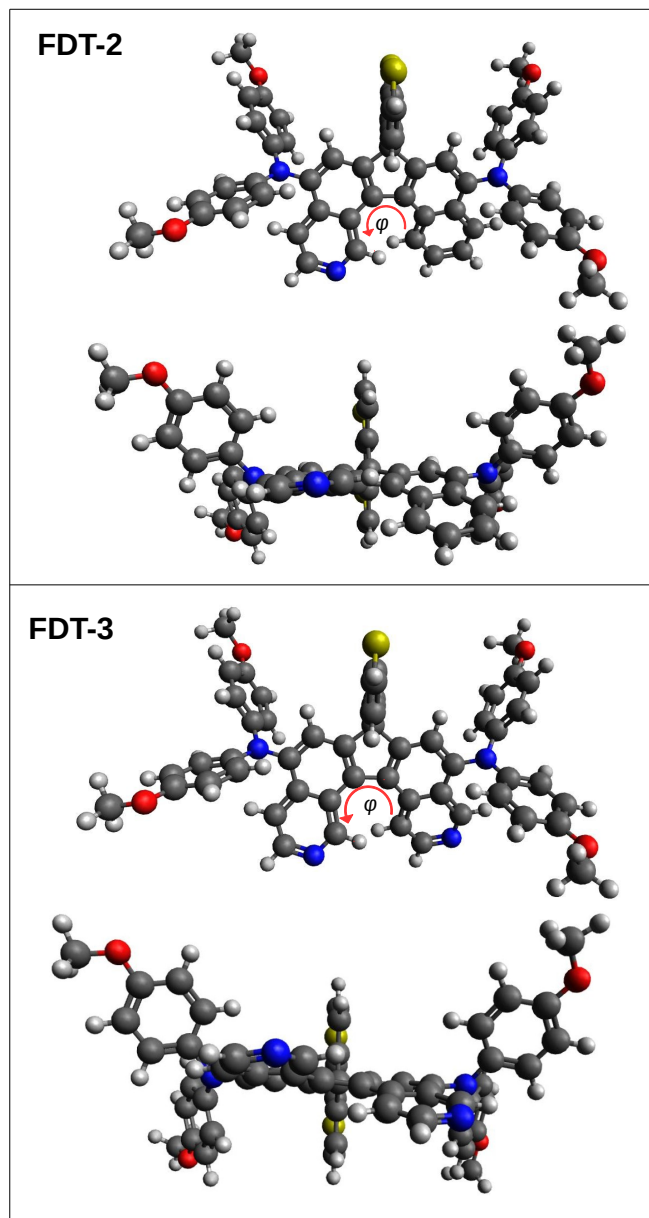


Figure S1: Optimized ground state geometries for **FDT-2** and **FDT-3** calculated at BMK/6-31G(d,p) level.

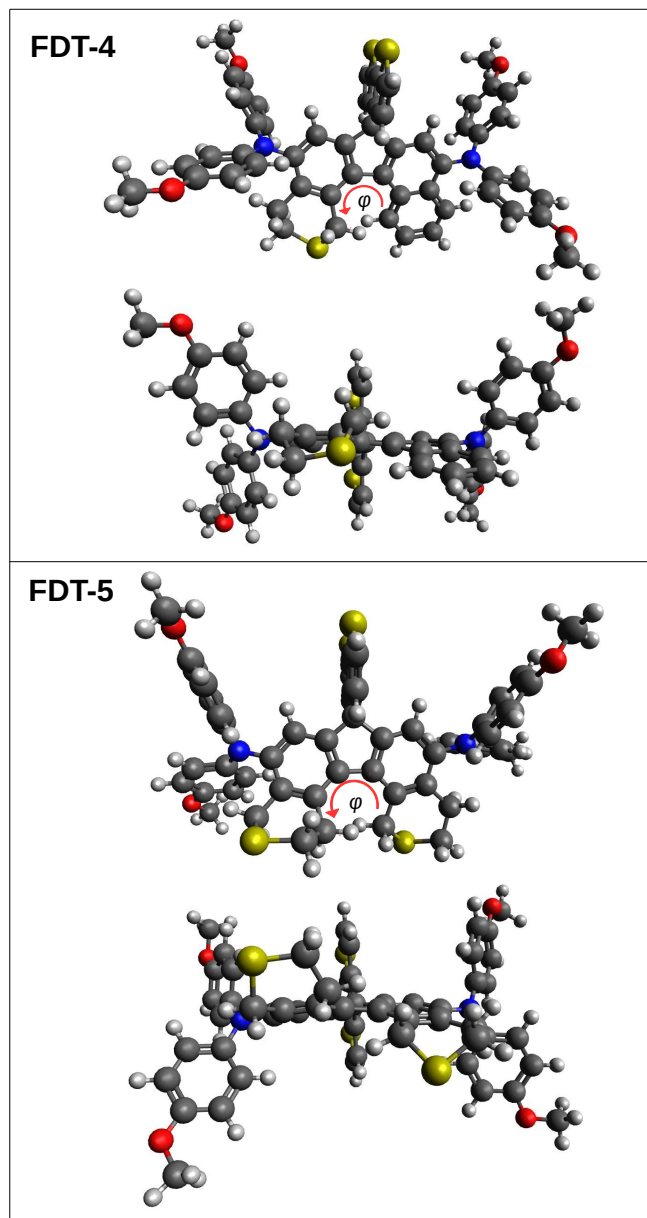


Figure S2: Optimized ground state geometries for **FDT-4** and **FDT-5** calculated at BMK/6-31G(d,p) level.

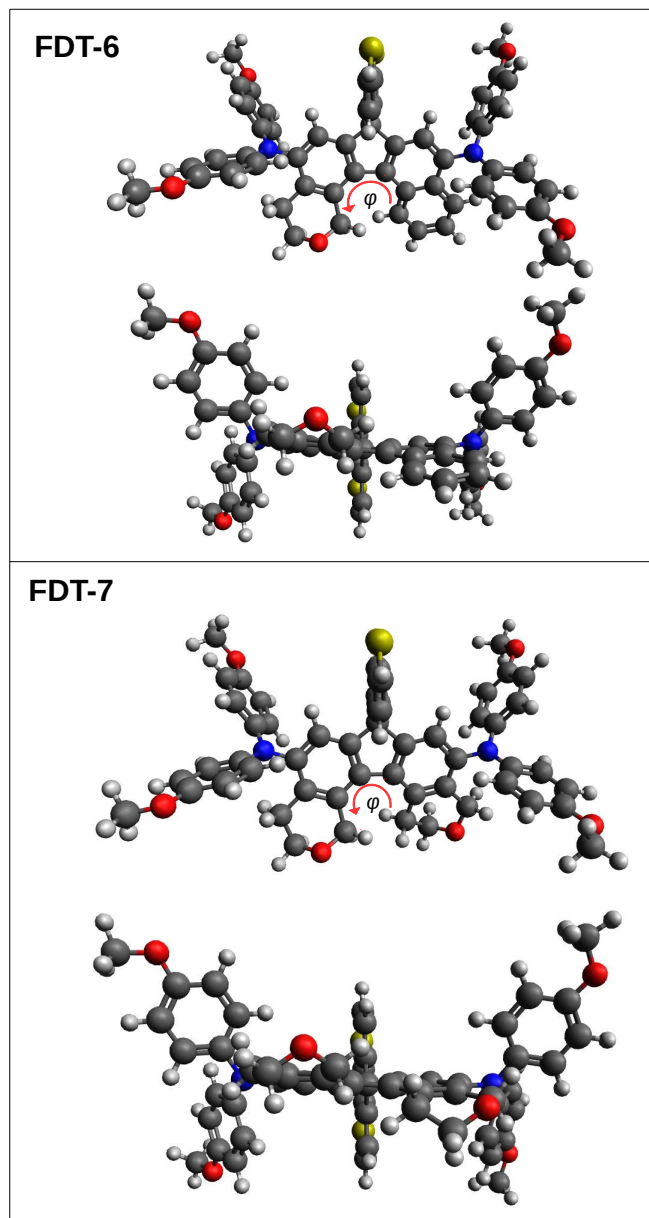


Figure S3: Optimized ground state geometries for **FDT-6** and **FDT-7** calculated at BMK/6-31G(d,p) level.

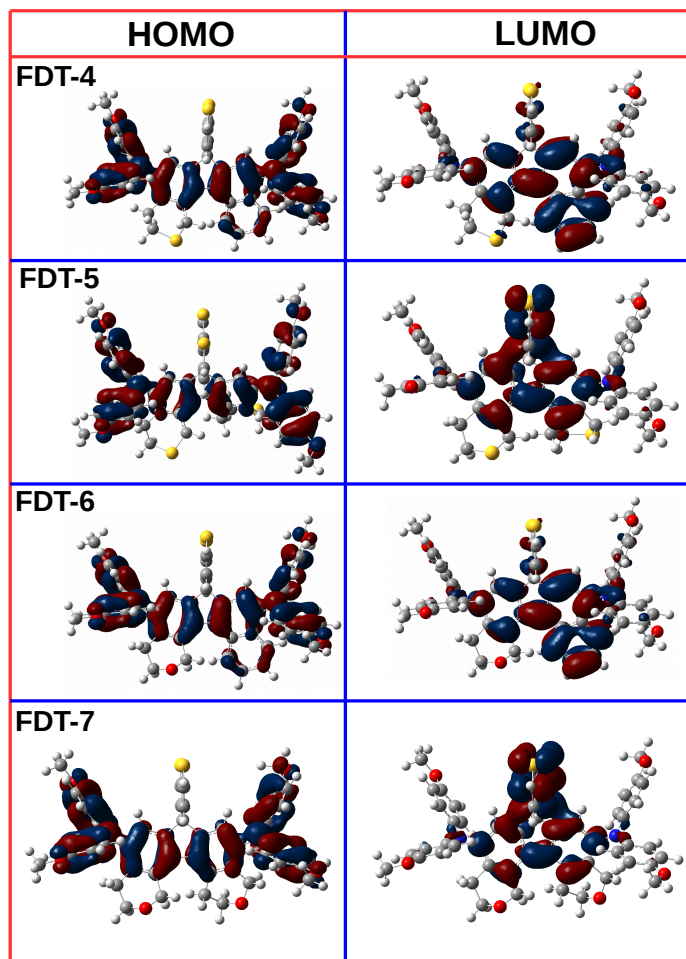


Figure S4: The spatial orbital distributions of HOMOs and LUMOs of **FDT-4** to **FDT-7** .

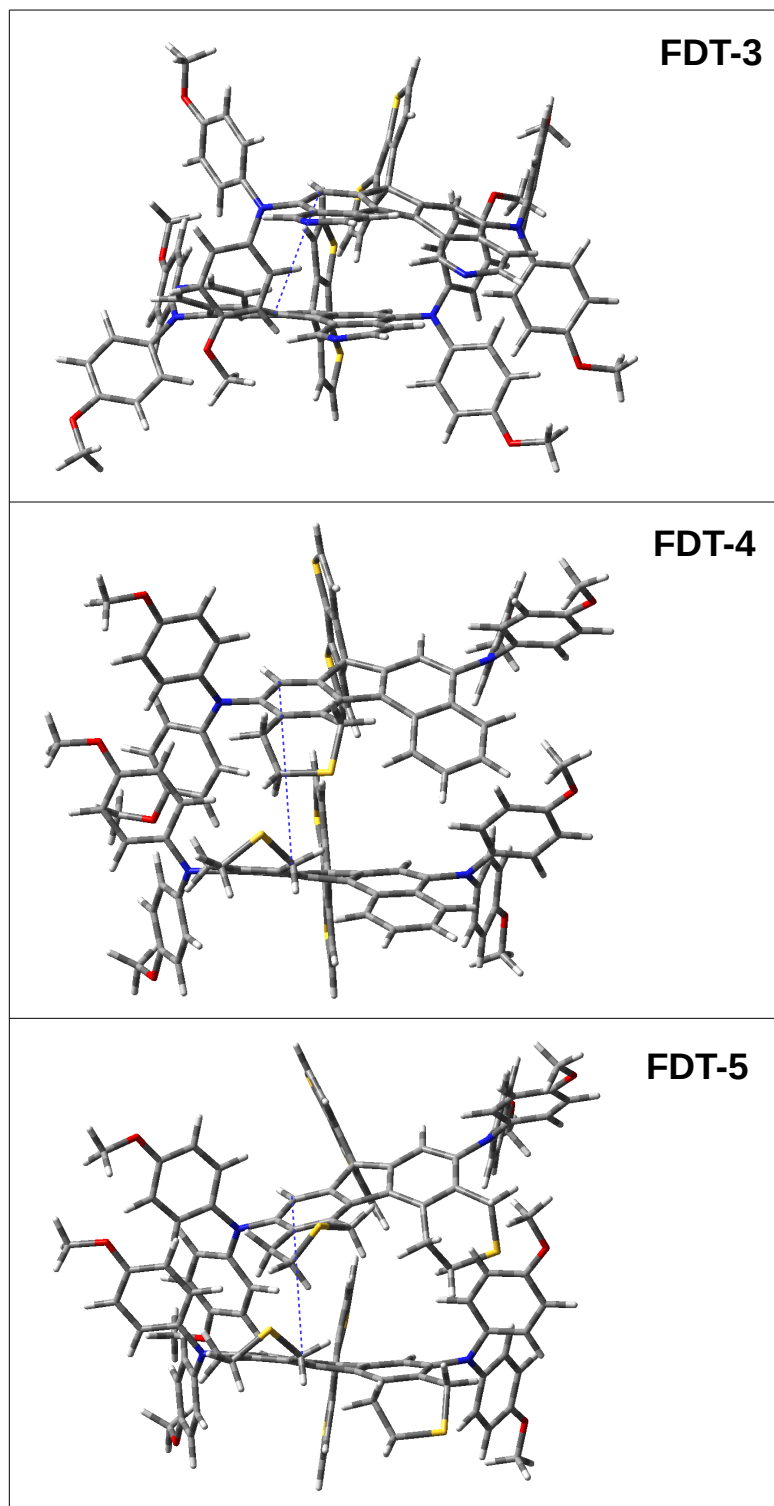


Figure S5: The π -stacked structures of two adjacent fragments for **FDT-3** to **FDT-5**.

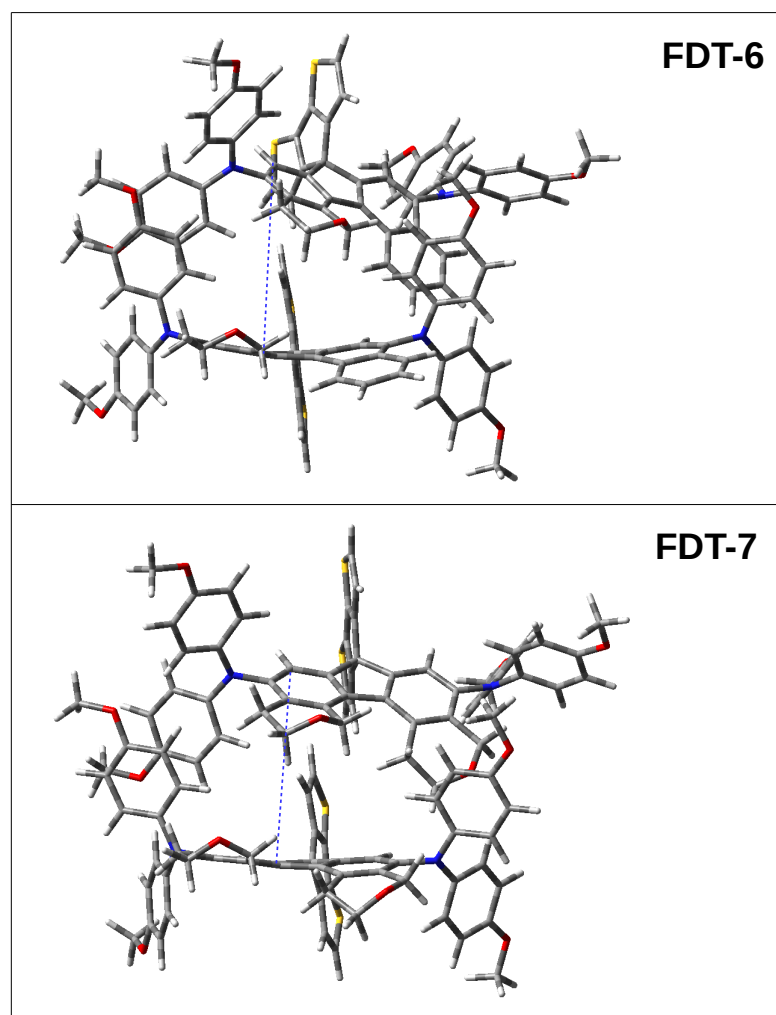


Figure S6: The π -stacked structures of two adjacent fragments for **FDT-6** to **FDT-7**.

References

- (1) Saliba, M.; Orlandi, S.; Matsui, T.; Aghazada, S.; Cavazzini, M.; Correa-Baena, J.-P.; Gao, P.; Scopelliti, R.; Mosconi, E.; Dahmen, K.-H., et al. A molecularly engineered hole-transporting material for efficient perovskite solar cells. *Nat. Energy* **2016**, *1*, 1–7.