

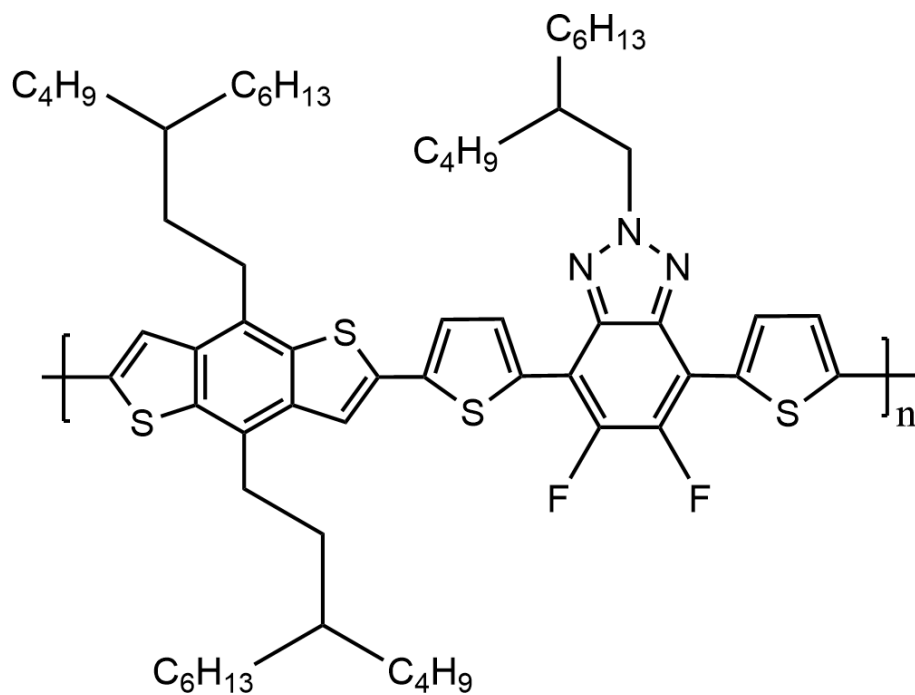
**Supporting Information:**

**Design and Screening of B-N Functionalized  
Non-fullerene Acceptors for Organic Solar Cells  
via Multiscale Computation**

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## FTAZ

Figure S1: Chemical structure of the FTAZ donor. Optimization of the donor polymer was performed at B3LYP/6-31G(d,p) level of theory considering one monomer unit.

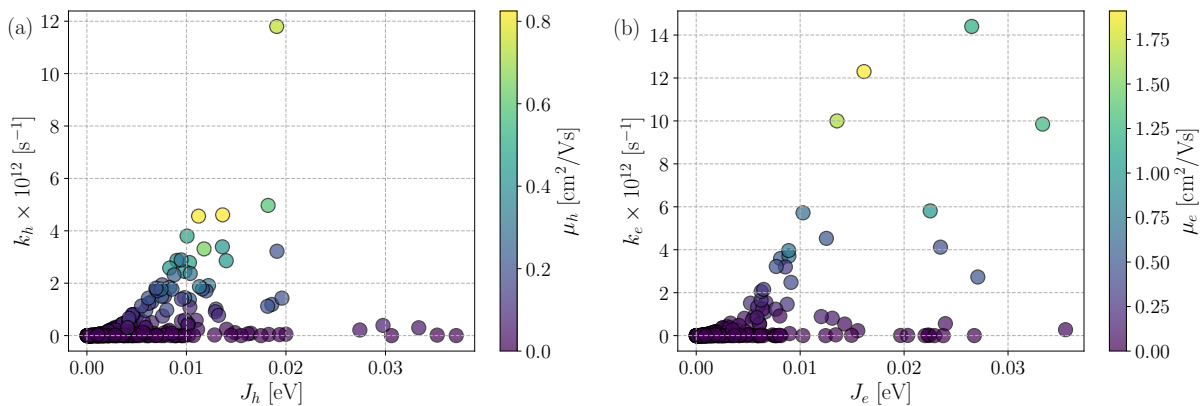


Figure S2: Correlation plot between the rate of charge transfer ( $k_h / k_e$ ) and electronic coupling ( $J_h / J_e$ ) for all the investigated eight thiophene systems: (a) holes and (b) electrons. The color of each point represents the charge carrier mobility ( $\mu_h / \mu_e$ ) value.

**Table S1: Comparison between predicted absorption wavelength ( $\lambda$ ) and electron mobility ( $\mu$ ) with experimental measurements.  $\lambda$  values are obtained at B3LYP/6-31G(d,p) level of theory.  $\mu$  was computed following the protocol described in Section 2.2 of the main manuscript.**

Compounds	$\lambda_{\text{sim}} [\text{nm}]$	$\lambda_{\text{exp}} [\text{nm}]$	$\mu_e (\text{sim}) (\text{cm}^2 \text{V}^{-1}\text{s}^{-1})$	$\mu_e (\text{exp}) (\text{cm}^2 \text{V}^{-1}\text{s}^{-1})$
INIC3	736	710 <sup>S1</sup>	$3.45 \times 10^{-2}$	$1.70 \times 10^{-4}$ <sup>S1</sup>
BCDT-4F	756	733 <sup>S2</sup>	$4.89 \times 10^{-2}$	$2.09 \times 10^{-4}$ <sup>S2</sup>
BCDT-4Cl	769	748 <sup>S2</sup>	$8.50 \times 10^{-2}$	$3.54 \times 10^{-4}$ <sup>S2</sup>

Table S2 of the supplementary information is provided in a separate excel sheet.

## References

- (S1) Dai, S.; Zhao, F.; Zhang, Q.; Lau, T.-K.; Li, T.; Liu, K.; Ling, Q.; Wang, C.; Lu, X.; You, W., et al. Fused nonacyclic electron acceptors for efficient polymer solar cells. *J. Am. Chem. Soc.* **2017**, *139*, 1336–1343.
- (S2) He, C.; Li, Y.; Li, S.; Yu, Z.-P.; Li, Y.; Lu, X.; Shi, M.; Li, C.-Z.; Chen, H. Near-infrared electron acceptors with unfused architecture for efficient organic solar cells. *ACS applied materials & interfaces* **2020**, *12*, 16700–16706.