Supporting Information

for

Understanding the Impact of Thiophene/Furan Substitution to Intrinsic Charge-Carrier Mobility

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Content

1. Benchmark Test

Table S1. Calculated and experimental hole reorganization energies (meV) of rubrene and pentacene

	Rubrene	**Pentacene**
Experimental	156[1]	100[2]
B3LYP/6-311G**	172	98
ωB97XD/6-311G**	253	171
M06-2X/6-31+G**	225	225
M06-HF/6-311G**	324	292

2. Potential Energy Surface (kcal/mol)

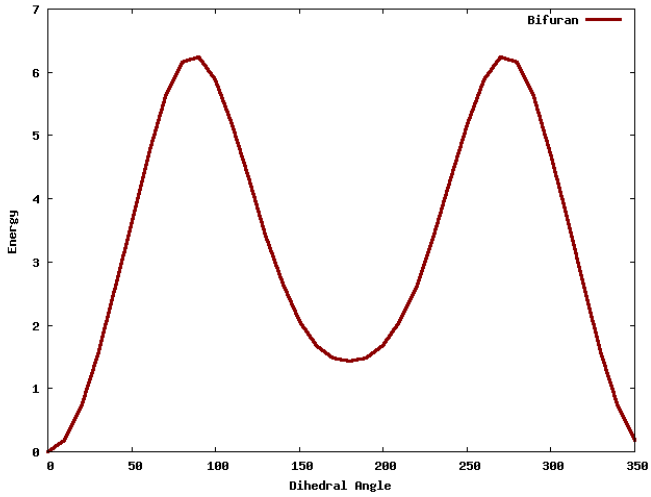


Fig S1. PES of bi-F at B3LYP/6-311G**

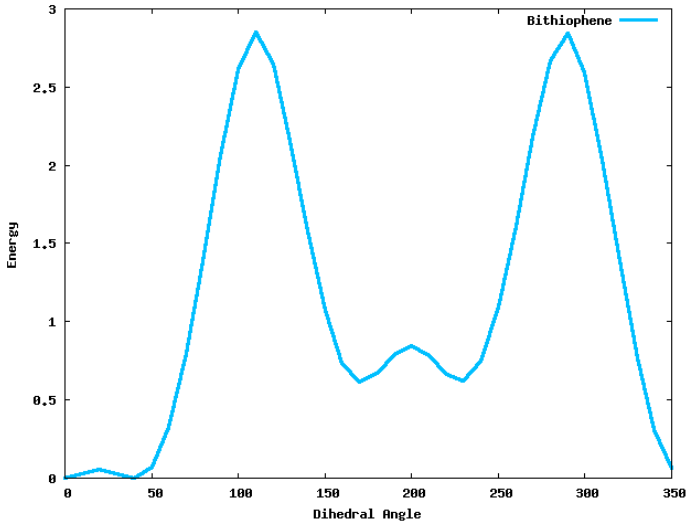


Fig S2. PES of bi-T at B3LYP/6-311G**

3. Single and double C-C bond lengths and Bond Length Alternation (BLA)

Table S2. BLA of Bi-F (Å) at B3LYP/6-311G**

Bi-F	Single Bonds	Double Bonds	BLA
	1.450	1.374	
	1.418	1.373	
	1.431	1.373	
	1.418	1.374	
	1.450		
Average	1.434	1.373	0.061

Table S3. BLA of Bi-T (Å) at B3LYP/6-311G**

Bi-T	Single Bonds	Double Bonds	BLA
	1.462	1.377	
	1.412	1.379	
	1.444	1.379	
	1.412	1.377	
	1.462		
Average	1.439	1.378	0.061

4. HOMO-LUMO of bi-F and bi-T monomers and dimers

Monomers

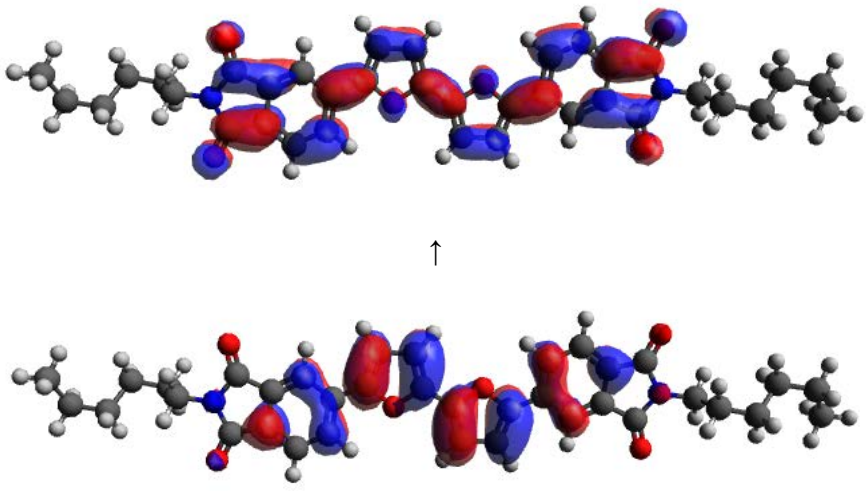


Figure S3A. HOMO and LUMO of bi-F at B3LYP/6-311G**

	eV	nm	f	Transition	c
bi-F	2.6859	461.62	1.2785	HOMO → LUMO (%99)	0.70

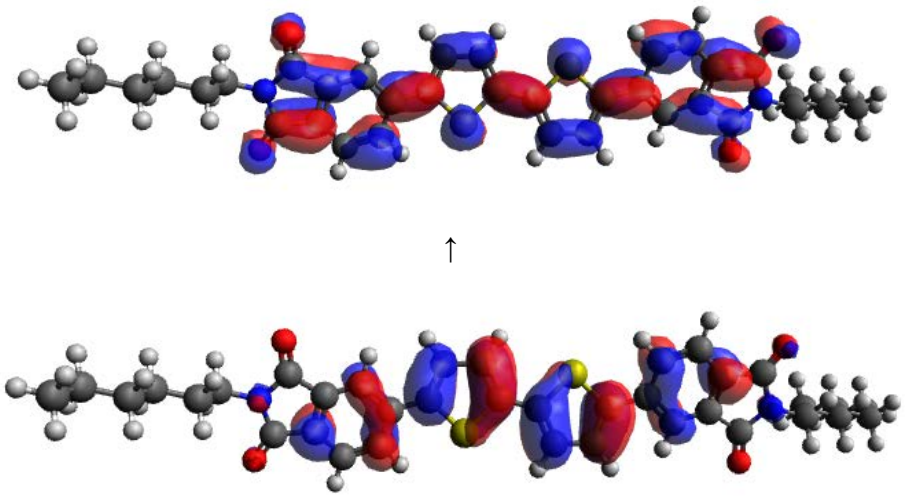


Figure S3B. HOMO and LUMO of bi-T at B3LYP/6-311G**

	eV	nm	f	Transition	c
bi-T	2.6929	460.40	1.3483	HOMO → LUMO (%99)	0.70

Dimers

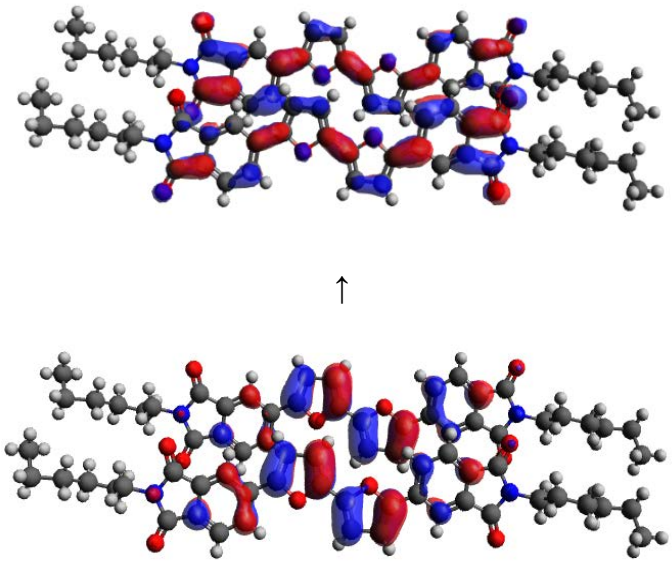


Figure S4A. HOMO-1 and LUMO of bi-F at B3LYP/6-311G**

	eV	nm	f	Transition	c
bi-F	2.7801	445.98	1.8710	HOMO-1 → LUMO (%72)	0.60

($S_O \rightarrow S_4$)				HOMO → LUMO+1 (%25)	0.35

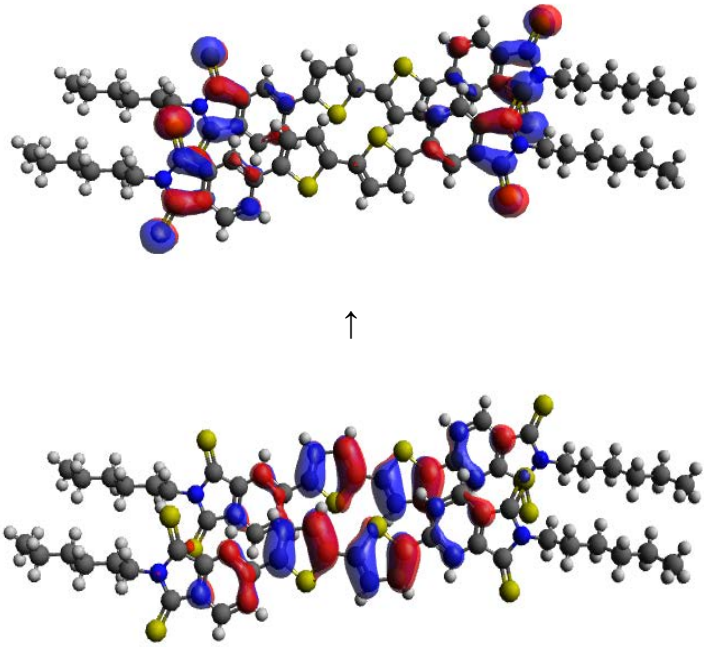


Figure S4B. HOMO-1 and LUMO of bi-T at B3LYP/6-311G**

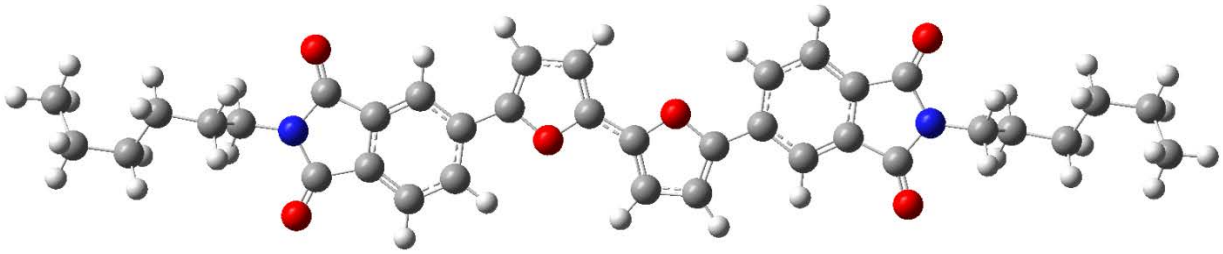
	eV	nm	f	Transition	c
bi-T ($S_O \rightarrow S_4$)	3.0684	404.07	1.4935	HOMO-1 → LUMO (%87) HOMO → LUMO+1 (%8) HOMO → LUMO+3 (%2)	0.66 0.20 0.11

Table S4. Calculated orbital energies of the derivatives at B3LYP/6-311G**

	Monomer bi-F	Monomer bi-T	Dimer bi-F	Dimer bi-T
LUMO+3	-1.58	-1.62	-2.43	-2.38
LUMO+2	-1.78	-1.96	-2.48	-2.50
LUMO+1	-2.44	-2.49	-2.78	-2.71
LUMO	-2.77	-2.89	-2.81	-2.71
HOMO	-5.75	-5.88	-5.73	-5.99
HOMO-1	-7.04	-7.09	-5.87	-6.15
HOMO-2	-7.51	-7.50	-6.95	-6.98
HOMO-3	-7.51	-7.52	-7.02	-7.16

5. Optimized Structures

Bi-F



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O	-3.55577900	5.21677100	6.55820900
C	0.24262600	0.23248400	0.63151700
C	1.42370600	0.05522100	1.30742800
H	2.26805200	-0.52129100	0.96771400
C	1.29961300	0.77589700	2.52235600
H	2.04203500	0.85597300	3.29972500
C	0.05401600	1.35385600	2.52524600
C	-0.65240600	2.19762700	3.47101200
C	-1.96463400	2.63819000	3.20077700
H	-2.43362200	2.33359000	2.27461200
C	-2.66212200	3.44964100	4.09410300
H	-3.67030900	3.78237600	3.87811500
C	-2.02689200	3.81901400	5.26824100
C	-0.73002000	3.38819600	5.54464100
C	-0.02538800	2.58522700	4.67497200
H	0.98088300	2.26783800	4.91904000

C	-2.49353300	4.66115800	6.40473900
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C	-1.45148600	5.42103500	8.58004300
H	-2.49683100	5.47172300	8.88618400
H	-0.89771600	4.82739400	9.31141400
C	-0.84019900	6.82365800	8.46363800
H	0.17442300	6.72343300	8.06637500
H	-1.41767800	7.40150400	7.73342200
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H	-0.20996100	6.98542100	10.52059800
H	-0.21890800	8.50392200	9.64870800
C	-2.16030000	7.93457800	10.38791400
H	-2.71210400	7.02046500	10.63857000
H	-2.74976900	8.44196500	9.61470000
C	-2.10077200	8.83207900	11.63395100
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H	-0.41319200	7.91900000	12.69117200
H	-1.98816600	7.25087400	13.13040600
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O	-0.71737000	-3.80171700	-7.46818600
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C	-1.42370600	-0.05522100	-1.30742800
H	-2.26805200	0.52129100	-0.96771400
C	-1.29961300	-0.77589700	-2.52235600
H	-2.04203500	-0.85597300	-3.29972500

C	-0.05401600	-1.35385600	-2.52524600
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C	1.96463400	-2.63819000	-3.20077700
H	2.43362200	-2.33359000	-2.27461200
C	2.66212200	-3.44964100	-4.09410300
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C	2.02689200	-3.81901400	-5.26824100
C	0.73002000	-3.38819600	-5.54464100
C	0.02538800	-2.58522700	-4.67497200
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H	-0.17442300	-6.72343300	-8.06637500
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C	0.78628100	-7.57803500	-9.80068800
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H	0.21890800	-8.50392200	-9.64870800
C	2.16030000	-7.93457800	-10.38791400
H	2.71210400	-7.02046500	-10.63857000
H	2.74976900	-8.44196500	-9.61470000
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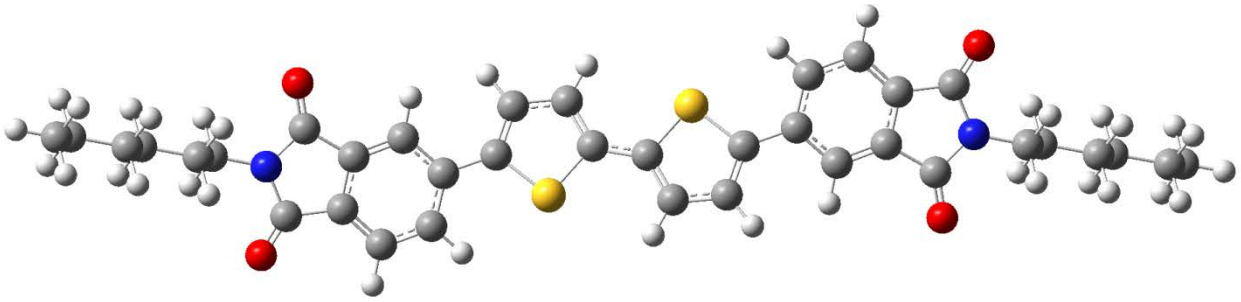
HF = -1954.93903018 a.u.

Bi-T



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HF = -2600.89747062 a.u.

References

S1. S. Duhm *et al.* Adv. Mater. 2012, 24, 901–905
S2. S. Kera *et al.* J. Phys. Chem. C 2013, 117, 22428−22437