Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Computational study on optical and NLO properties of Donor-Acceptor interaction molecules containing triazolobenzothiadiazole or benzothiadiazole central acceptor core

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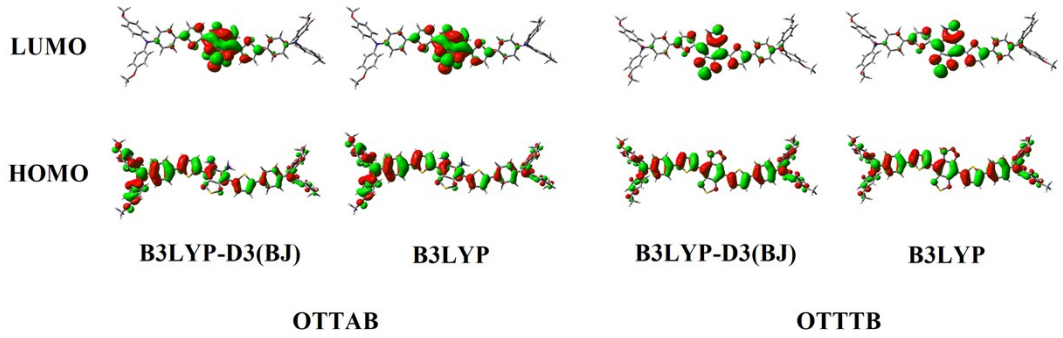


Fig.S1 The contour plots of the HOMO and LUMO for OTTAB and OTTTB using the B3LYP-D3(BJ) and B3LYP functionals.

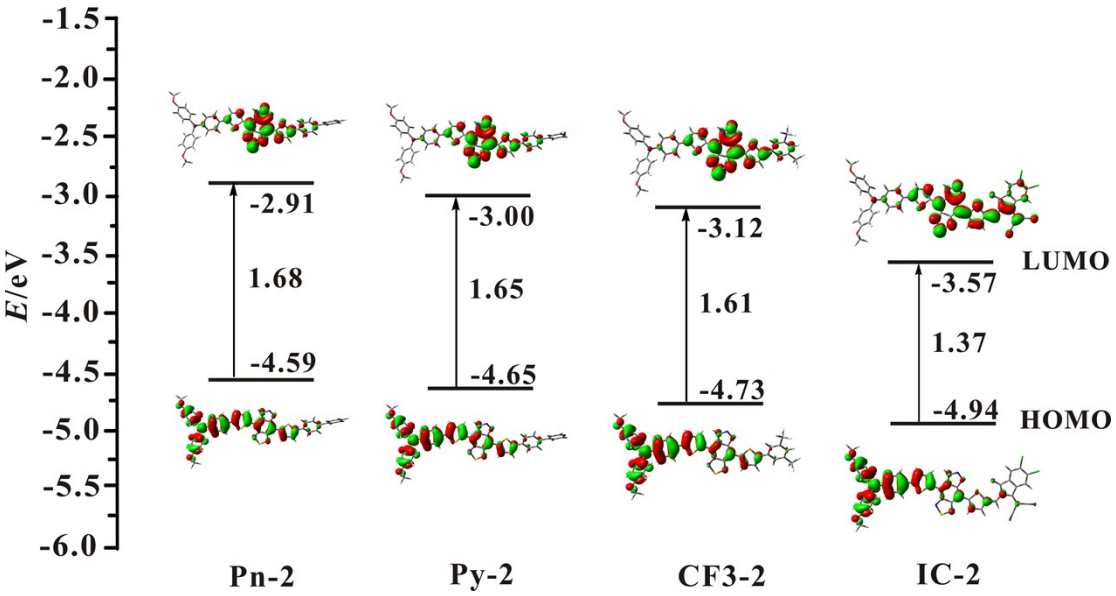
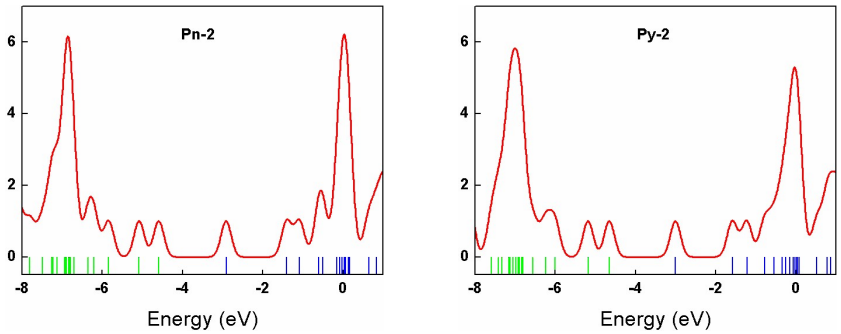


Fig. S2. Energy levels and frontier molecular orbital diagram of Pn-2, Py-2, CF3-2 and IC-2



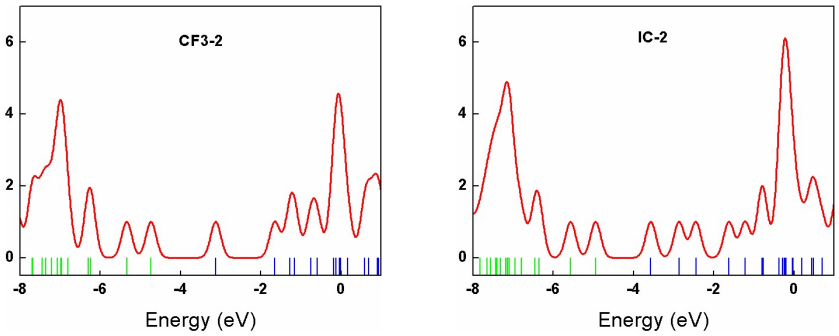


Fig. S3. DOS spectra of Pn-2, Py-2, CF3-2 and IC-2

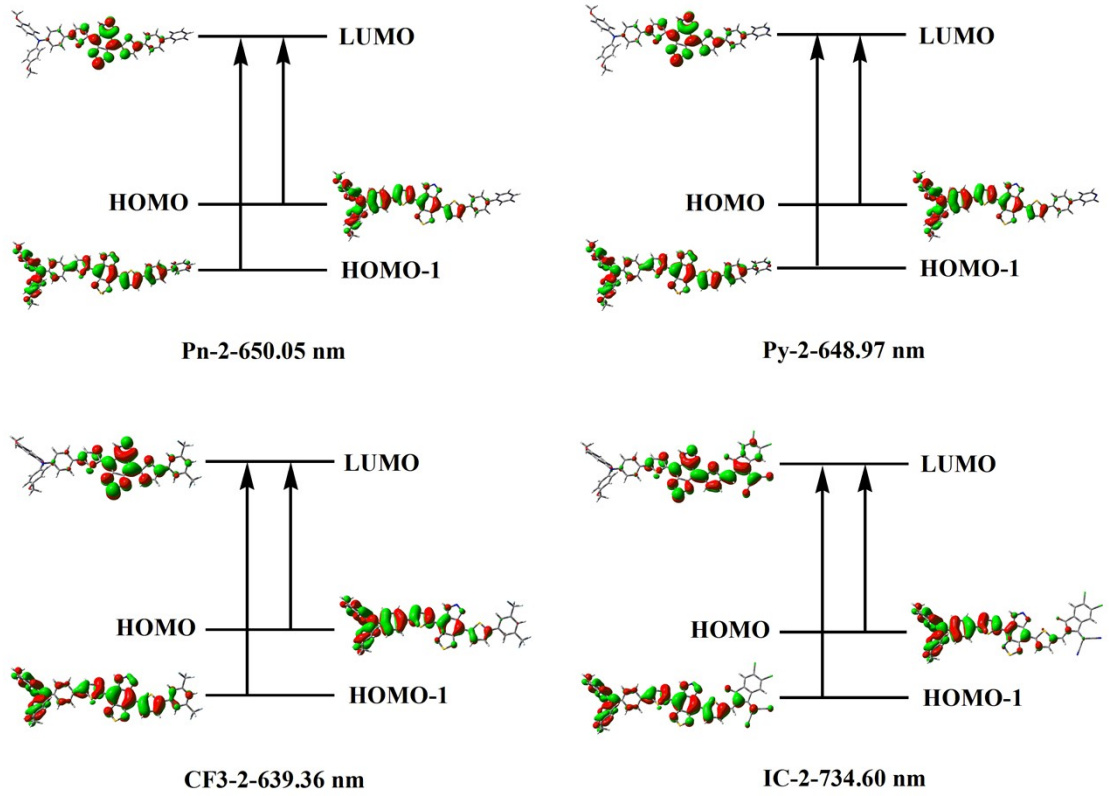
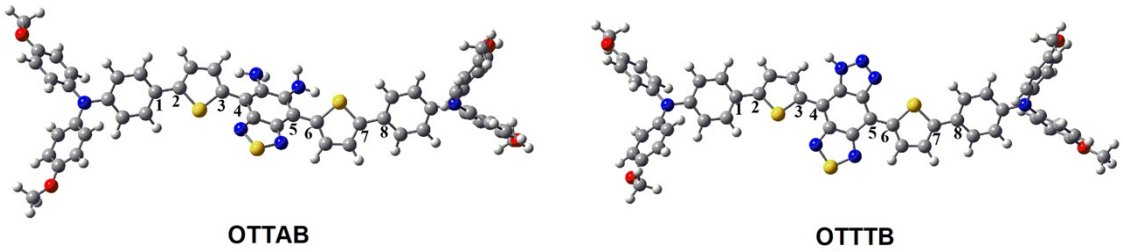


Fig. S4. Molecular orbital isosurfaces involved in the main electron transitions of Pn-2, Py-2, CF3-2 and IC-2 at the CAM-B3LYP/6-31+G(d) level of theory.

Table S1 The selected bond lengths, the HOMO/LUMO energy level and energy gap (Eg) for OTTAB and OTTTB using the B3LYP-D3(BJ) and B3LYP functional.



Schematic diagram of chemical structure of OTTAB and OTTTB.

(a)

OTTAB	C1-C2	C3-C4	C5-C6	C7-C8	HOMO	LUMO	Eg

B3LYP-D3(BJ)	1.460	1.459	1.463	1.460	-4.44	-1.92	2.52
B3LYP	1.463	1.464	1.468	1.468	-4.48	-1.89	2.59
(b)							
OTTTB	C1-C2	C3-C4	C5-C6	C7-C8	HOMO	LUMO	Eg
B3LYP-D3(BJ)	1.458	1.445	1.437	1.456	-4.39	-2.76	1.63
B3LYP	1.462	1.450	1.441	1.459	-4.42	-2.75	1.67

Table S2. The calculated β_{HRS} values ($\times 10^{-30}$ esu) of the OTTAB, OTTTB, Pn-1, Py-1, CF3-1 and IC-1 by using different functionals associated with the 6-31+G(d) basis set.

Derivative	B3LYP	CAM-B3LYP	BHandHLYP	LC-BLYP	CAM-B3LYP（THF）
OTTAB	36.31	14.69	16.23	9.28	21.91
OTTTB	141.45	98.48	90.63	69.42	171.95
Ph-1	606.39	221.49	229.33	125.77	376.22
Py-1	729.38	269.01	282.87	152.36	448.73
CF3-1	776.32	311.34	327.57	180.69	537.00
IC-1	1827.02	866.01	874.80	568.865	2064.45