Supporting Information

For the Article entitled

Theoretical studies to investigate the effect of different cores and two different topologies on the optical and charge transfer properties of donor materials for organic solar cells.

Shamsa Bibi [ab] and Jingping Zhang[c]*

School of Chemistry, Northeast Normal University, Changchun, P.R. China [a],

Faculty of Chemistry, University of Agriculture Faisalabad, Pakistan [b],

Faculty of Chemistry, Northeast Normal University [c], Changchun 130024, P.R. China

*Corresponding author:

Prof. Jingping Zhang

E-mail: jpzhang@nenu.edu.cn

Tel: +86-431-85099372

Fax: +86-431-85684937

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SI: Optimized Geometry Structures for the Designed Donor Molecules

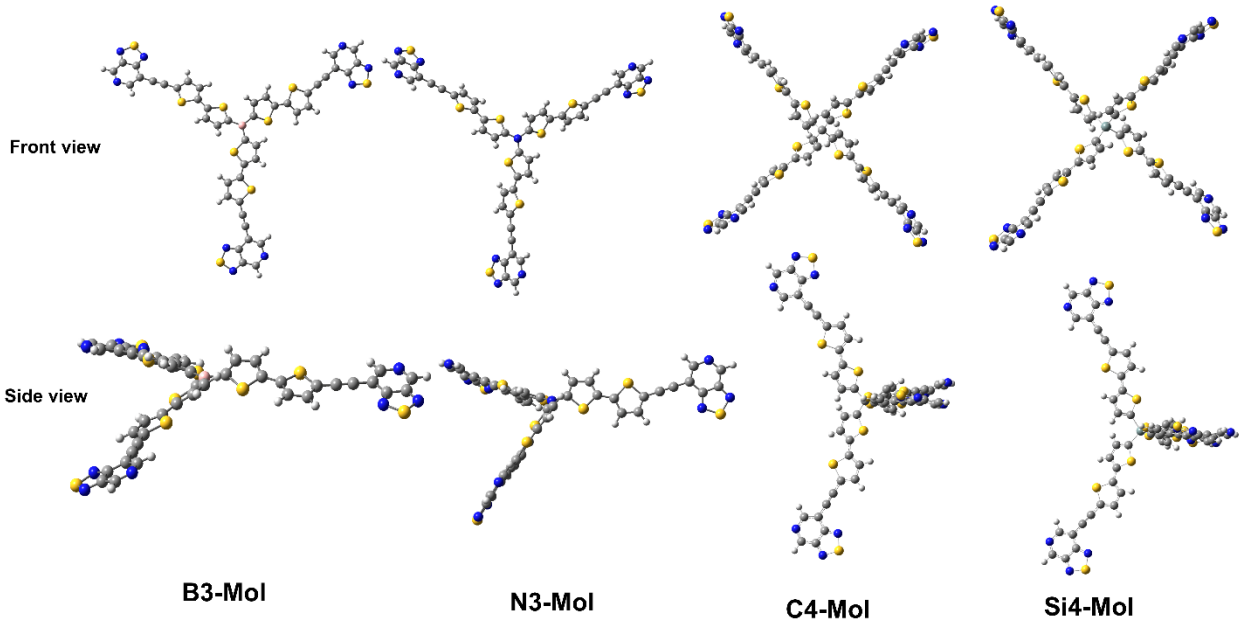

Figure S1a. Optimized geometry structures of the "core-D-π-A" topology based three (C3 symmetry) and four arms (C2 symmetry) designed molecules.

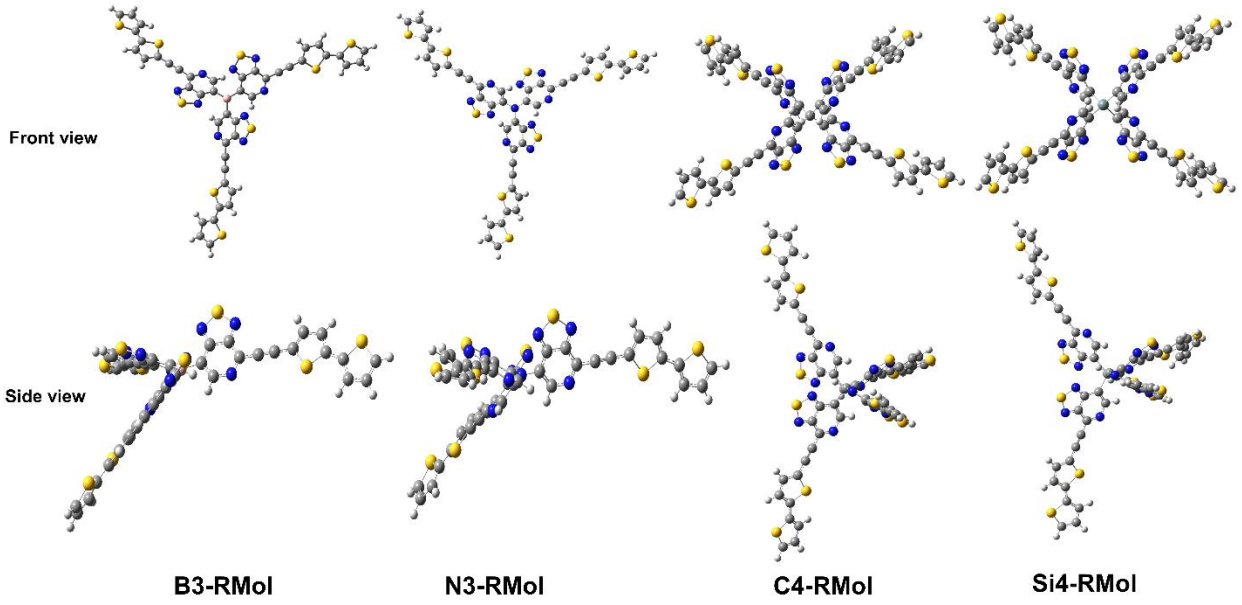

Figure S1b. Optimized geometry structures of the "core-A-π-D" topology based three (C3 symmetry) and four arms (C2 symmetry) designed molecules

SII: Frontier Molecular orbitals (FMOs) of three and four arms Designed Donor Molecules

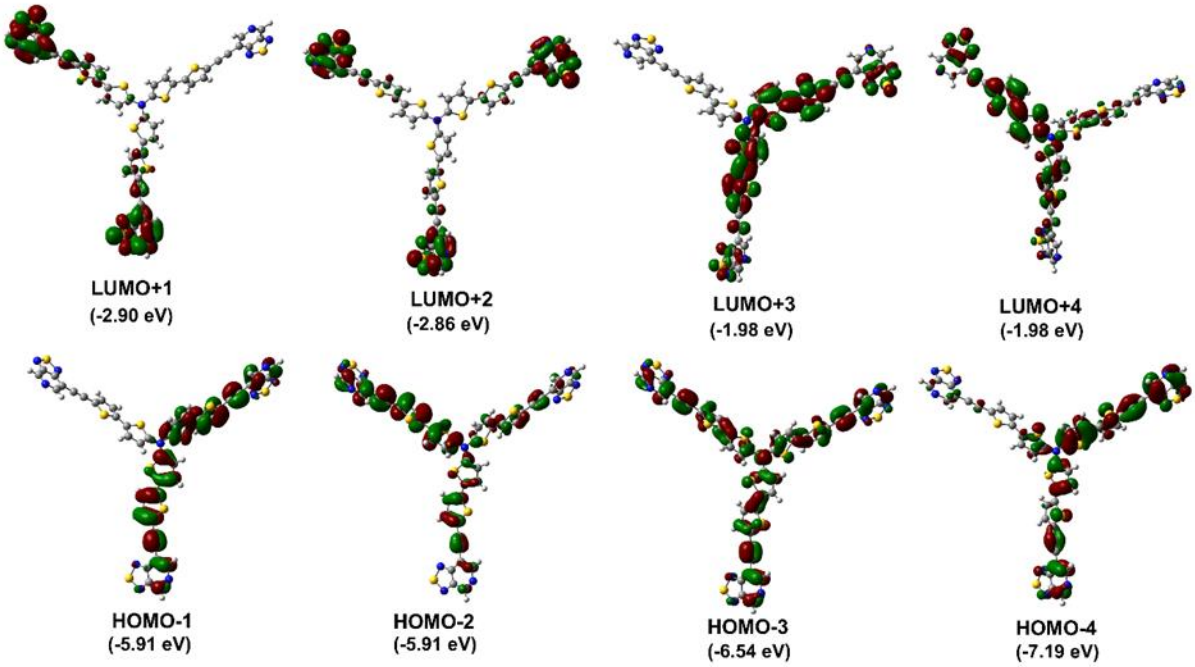

Figure S2a. FMOs of the **N3-Mol**.

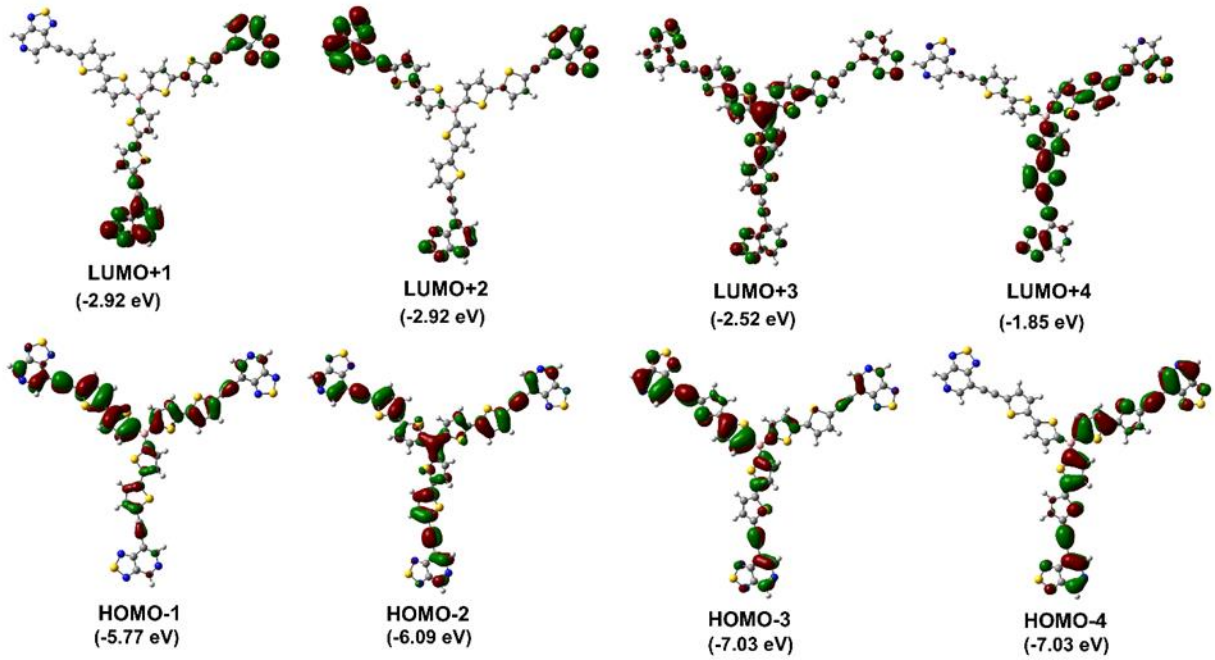

Figure S2b. FMOs of the **B3-Mol**.

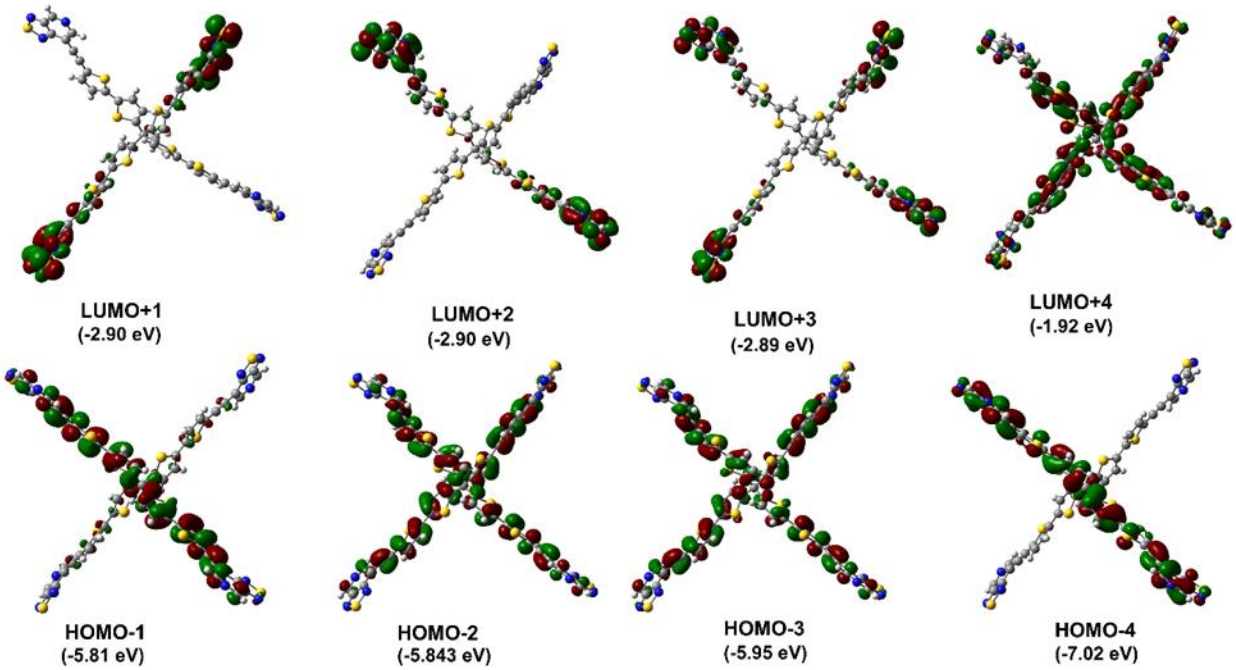

Figure S2c. FMOs of the **C4-Mol**.

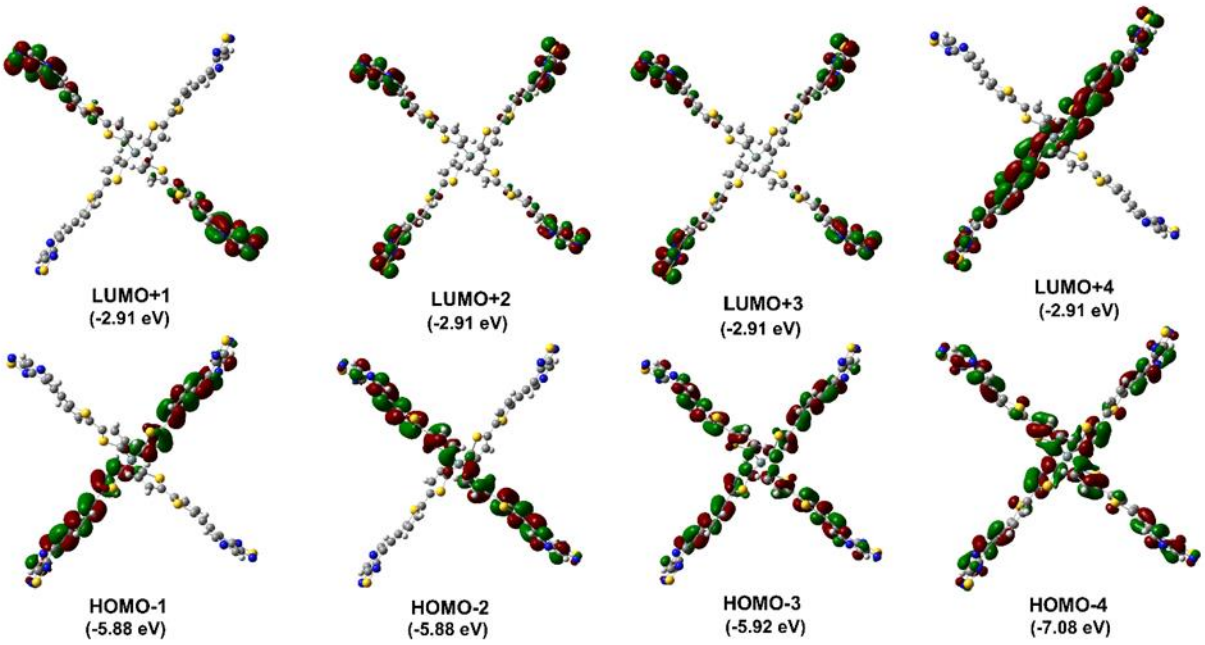

Figure S2d. FMOs of the **Si4-Mol**.

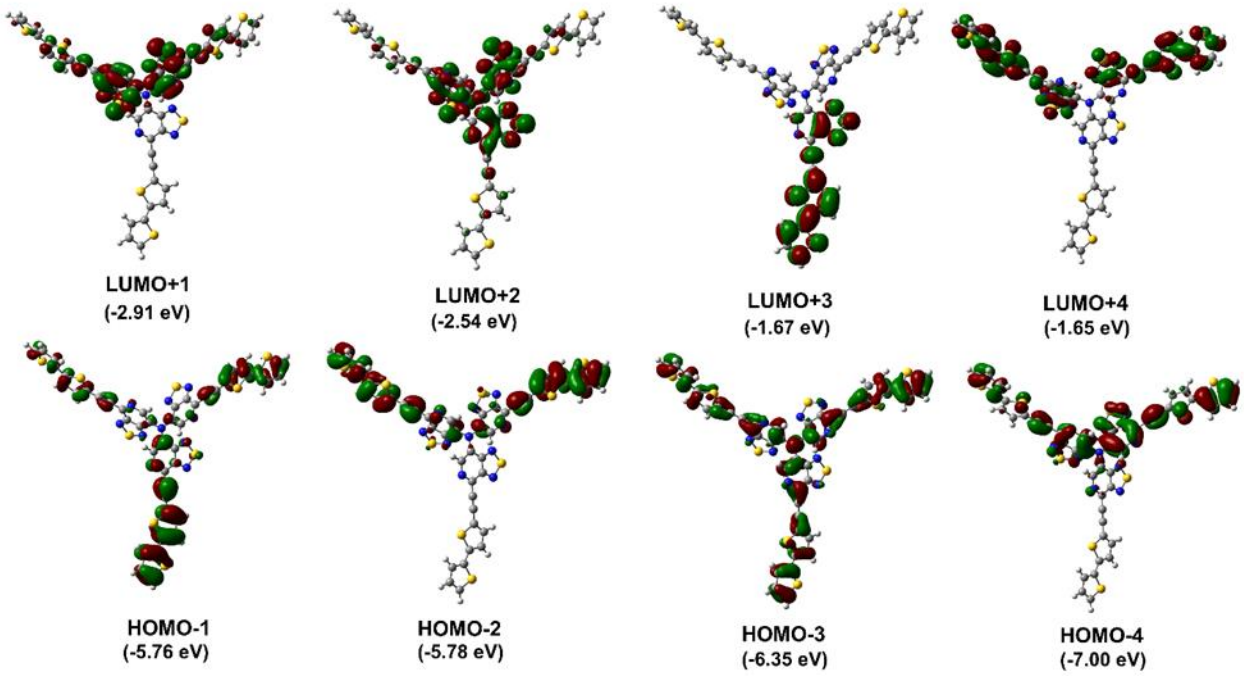

Figure S2e. FMOs of the **N3-RMol**.

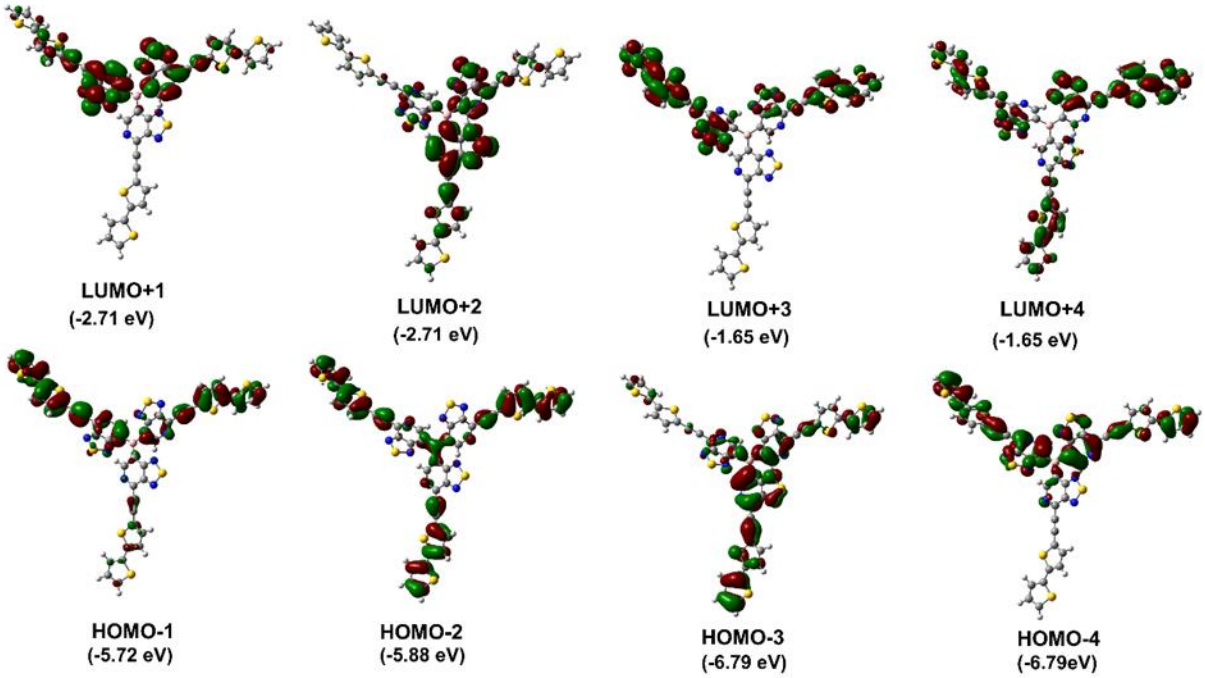

Figure S2f. FMOs of the **B3-RMol**.

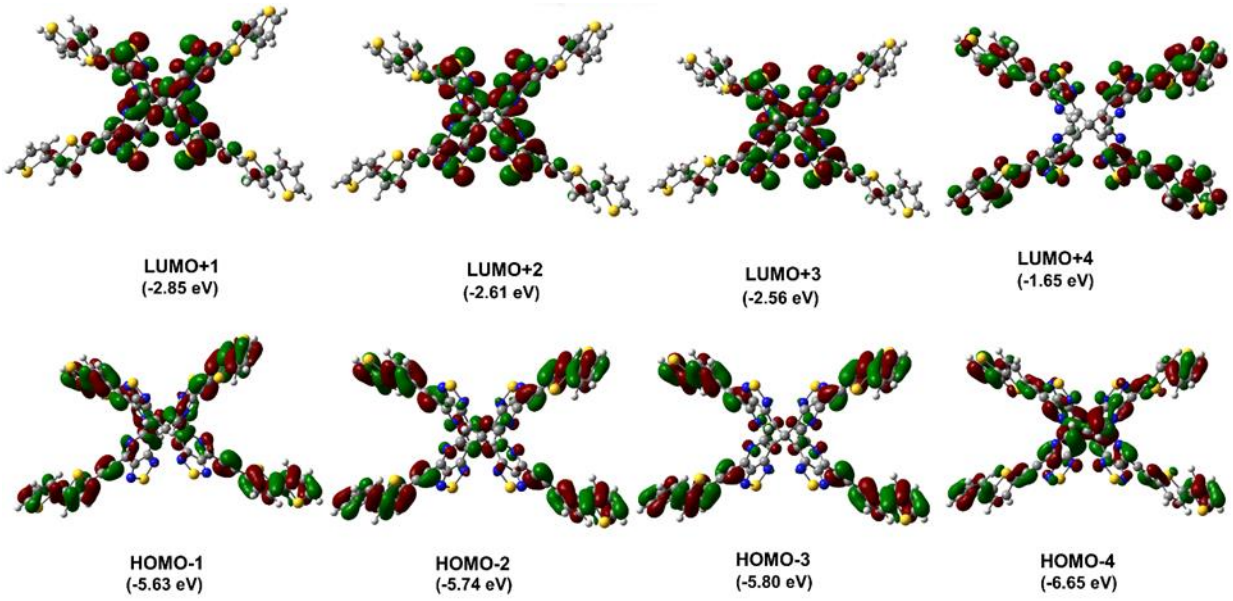

Figure S2g. FMOs of the **C4-RMol**.

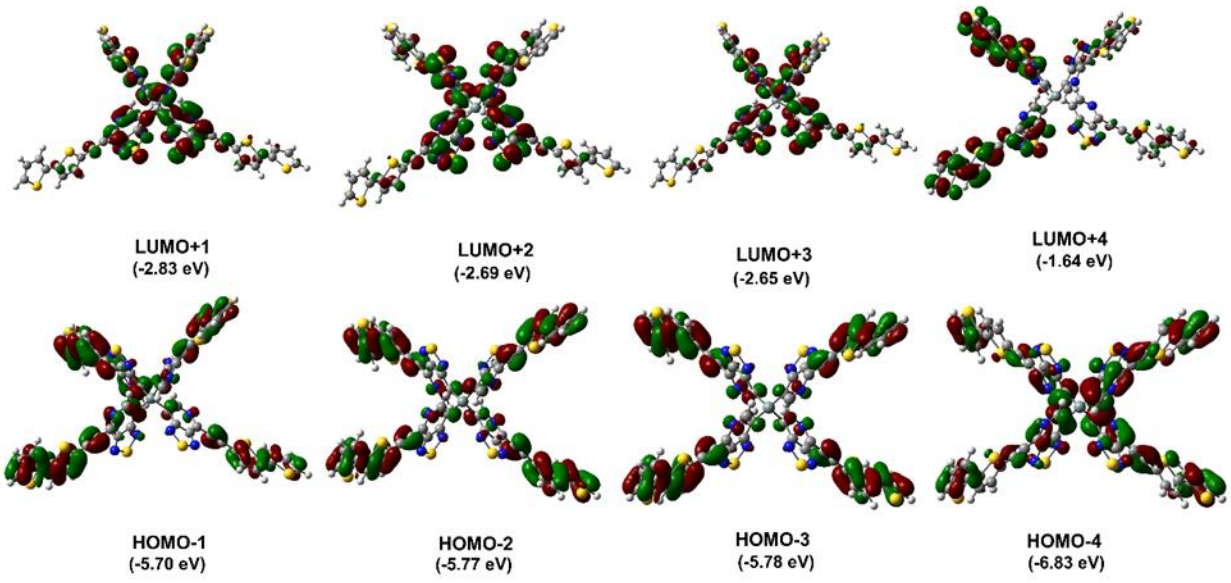

Figure S2h. FMOs of the **Si4-RMol**.

SIII. FMOs Energy Data of the three and four arms Designed Donor Molecules

Table S1. Calculated energy data (in eV) of the FMOs of the three and four arms designed donor molecules. (E_{HOMO} = HOMO energy levels; E_{LUMO} = LUMO energy levels; and Eg = E_{LUMO} - E_{HOMO}).

Name	E_{HOMO} (eV)	E_{LUMO} (eV)	Eg (eV)
C4-Mol	-5.81	-2.91	2.90
Si4-Mol	-5.84	-2.91	2.93
B3-Mol	-5.77	-3.02	2.75
N3-Mol	-5.26	-2.90	2.36
C4-RMol	-5.59	-2.94	2.65
Si4-RMol	-5.69	-2.84	2.85
B3-RMol	-5.71	-3.09	2.62
N3-RMol	-5.32	-2.91	2.41

SIV: Molecular Orbital Compositions (in percentage)

Table S2. Molecular orbital composition in percentage from π-spacer (Ps), donor (DF) and acceptor (AF) fragments for designed donor molecules.

Molecule	Energy Level	AF	Ps	DF
N3-Mol	HOMO	6.6	7.2	76
	LUMO	84.3	4.9	10.7
B3-Mol	HOMO	14	14.8	71.1
	LUMO	65.3	5.5	24
C4-mol	HOMO	15.1	15.7	68.5
	LUMO	85.5	4.9	9.6
Si4-Mol	HOMO	15.9	16.4	67.5
	LUMO	85.1	4.9	9.8
N3-RMol	HOMO	35.1	15.8	39.4

	LUMO	79.4	7.7	12.8
B3-RMol	HOMO	21.3	16	62.7
	LUMO	63	10.1	15.5
C4-RMol	HOMO	25	16.5	58.2
	LUMO	78.6	8.1	13.1
Si4-RMol	HOMO	18.4	16.1	65.4
	LUMO	77.7	8.0	13.7

SV: Absorption Properties

Table S3. Calculated excitation energies (Ex), wavelength (λ_{abs}), oscillator strength (*f*), and composition in terms of molecular orbitals with related character (H = HOMO, L = LUMO) for the designed donor molecules.

Donor	Transition state	Ex (eV)	λ_{abs} (nm)	*f* (a.u.)	Assignment
N3-Mol	S0→S1	2.03	610	0.62	H→L
	S0→S4	2.64	471	0.63	H→L+1
	S0→S7	2.77	447	0.41	H→L+3
	S0→S16	3.47	356	0.47	H-1→L+3, H-1→L+4.
B3-Mol	S0→S1	2.32	534	1.43	H→L
	S0→S8	2.83	437	0.30	H→L+3
	S0→S13	3.47	357	0.51	H-1→L+5, H→L+4.
C4-Mol	S0→S1	2.45	504	0.52	H→L , H→L+3
	S0→S2	2.46	503	0.97	H→L+2
	S0→S3	2.47	502	0.97	H-1→L, H-2→L+1
	S0→S17	3.35	370	0.59	H-2→L+4
	S0→S18	3.36	368	1.46	H→L+4
	S0→S24	3.53	350	0.12	H→L+4, H-2→L+5

Si4-Mol	S0→S1	2.48	499	0.61	H→L+1
	S0→S2	2.49	498	1.00	H→L
	S0→S17	3.32	373	0.68	H-1→L+4, H→L+6
	S0→S18	3.34	370	1.51	H→L+4, H-1→L+6
N3-RMol	S0→S1	1.90	649	0.80	H→L
	S0→S2	1.90	648	0.78	H→L+1
	S0→S4	2.46	504	0.39	H-1→L+1
	S0→S12	3.19	387	0.83	H→L+3
	S0→S20	3.68	337	0.14	H-1→L+3
	S0→S24	3.74	331	0.23	H-2→L+5, H-4→L+1
B3-RMol	S0→S1	2.30	562	1.07	H→L
	S0→S2	2.21	561	1.11	H-1→L
	S0→S4	2.58	481	0.44	H→L+2
	S0→S7	2.67	463	0.12	H-1→L+1, H→L+2
	S0→S16	3.56	348	0.43	H-1→L+4
C4-RMol	S0→S1	2.20	563	0.35	H→L
	S0→S2	2.25	551	1.21	H-1→L, H→L+1
	S0→S5	2.38	521	0.78	H-2→L
	S0→S14	2.73	453	0.34	H-2→L+3, H-3→L+2
	S0→S23	3.46	358	0.37	H→L+4
	S0→S25	3.47	357	0.14	H→L+5
Si4-RMol	S0→S1	2.41	513	1.56	H→L
	S0→S3	2.49	497	1.24	H-2→L, H-3→L+1
	S0→S11	2.68	462	0.30	H-2→L+2
	S0→S21	3.47	357	0.68	H-4→L+1, H-1→L+4
	S0→S23	3.52	351	0.71	H-3→L+4
	S0→S28	3.63	341	0.58	H→L+5

SVI: Chemical Structure of PCBM

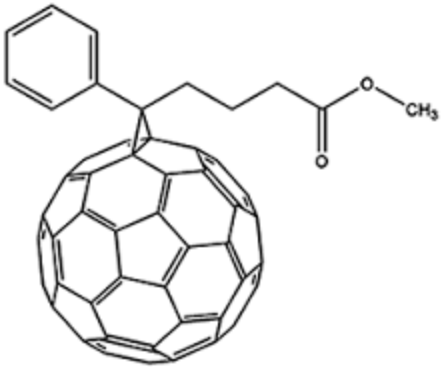

Figure S3. Chemical structure of acceptor molecule **PCBM.**

SVII: Stability

Table S4. Calculated η values in eV for investigated three and four arms molecules at the B3LYP/6-31G (d, p) level of theory.

Name	η	Name	η
C4-Mol	4.371	C4-RMol	4.341
Si4-Mol	4.352	Si4-RMol	4.300
B3-Mol	3.999	B3-RMol	3.920
N3-Mol	3.942	N3-RMol	3.910

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