Supporting Information

Computational Insights into Phthalimide-Core Non-Fullerene Acceptors for Next-Generation Organic Solar Cells

Zunaira Khan,[a] Hussain J. Alathlawi,[b] Karrar Hazim Salem,[c] Syed Muhammad Kazim Abbas Naqvi,*[d,e] Ines Hilali Jaghdam,[f] Mohamed S. Soliman,[g] Tamer H. A. Hasanin,[h] Sajjad Ali,[a] Haq Nawaz Bhatti,*[a] Rasheed Ahmad Khera,*[a]

[a]Department of Chemistry, University of Agriculture, Faisalabad, Pakistan
[b]Department of Physical Sciences, Physics Division, College of Science, Jazan University, P.O. Box. 114, Jazan 45142, Kingdom of Saudi Arabia
[c]College of Medical and Health Technologies, Al-Zahraa University for Women, Karbala, Iraq
[d]Faculty of Materials Science, Shenzhen MSU-BIT University, Shenzhen, 518115, China.
[e]Platform for Applied Nanophotonics, Institute of Advanced Interdisciplinary Technology, Shenzhen MSU-BIT University, Shenzhen, 518115, China
[f]Department of Computer Science and Information Technology, Applied College., Princess Nourah bint Abdulrahman University, P.O. Box 84428, Riyadh 11671, Saudi Arabia
[g]Department of Electrical Engineering, College of Engineering, Taif University, Taif, 21944, Saudi Arabia
[h]Department of Chemistry, College of Science, Jouf University, P.O. Box 2014, Sakaka, Saudi Arabia

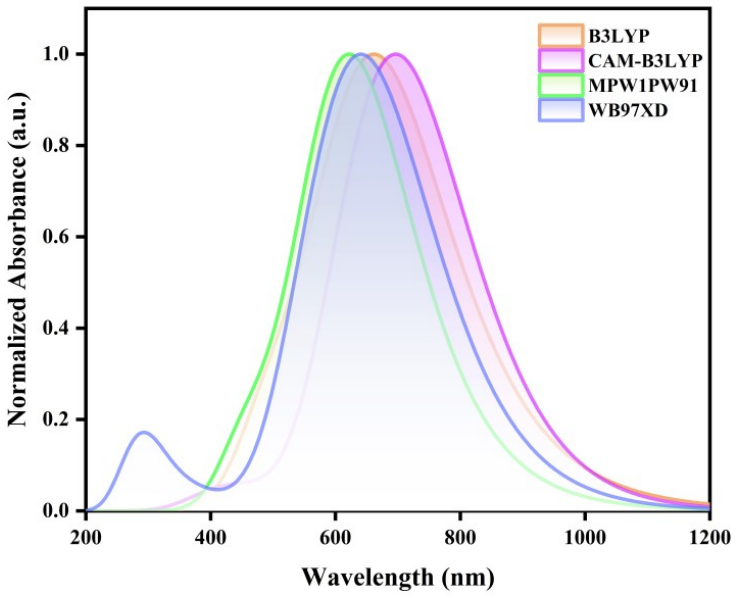

Figure S1 Comparison of four distinct functionals (B3LYP, CAMB3LYP, WB97XD, and MPW1PW91)

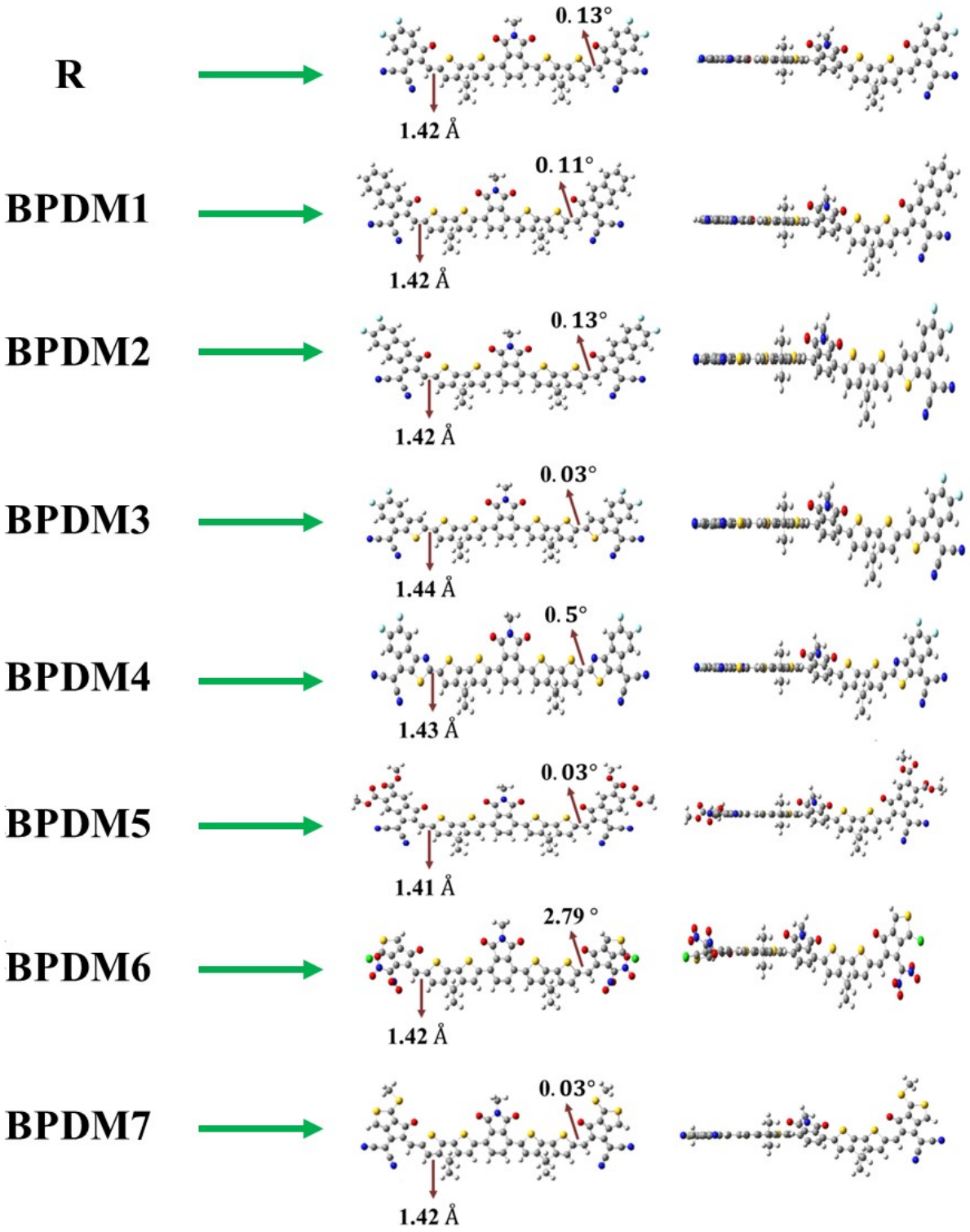

Figure S2 Optimized geometries of R and BPDM1-BPDM7 illustrating interatomic distances and torsional angles

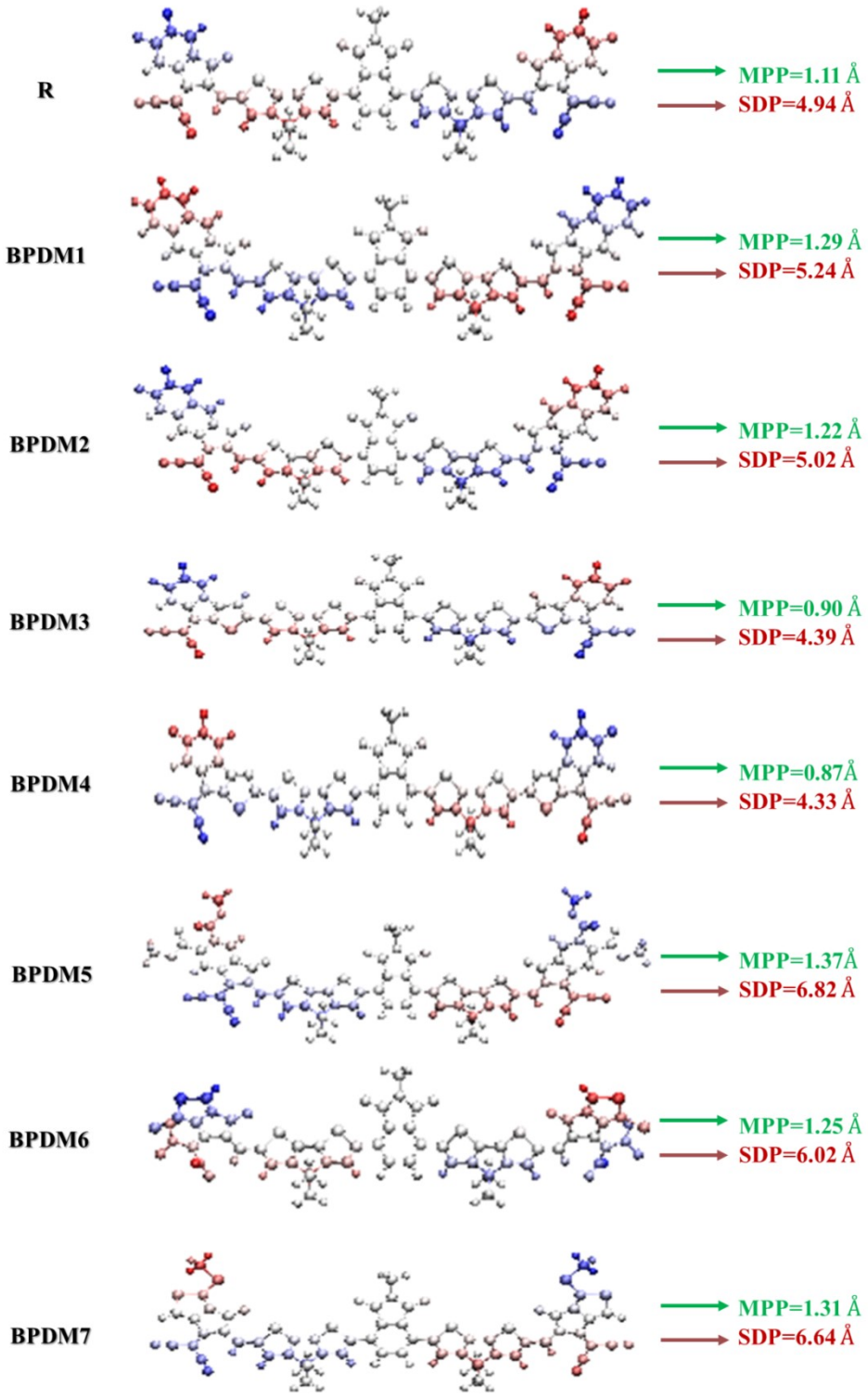

Figure S3 Visualization of molecular planarity in R and BPDM1-BPDM7 based on MPP (Molecular Planarity Parameter) and SDP (Span of Deviation from the Plane) values

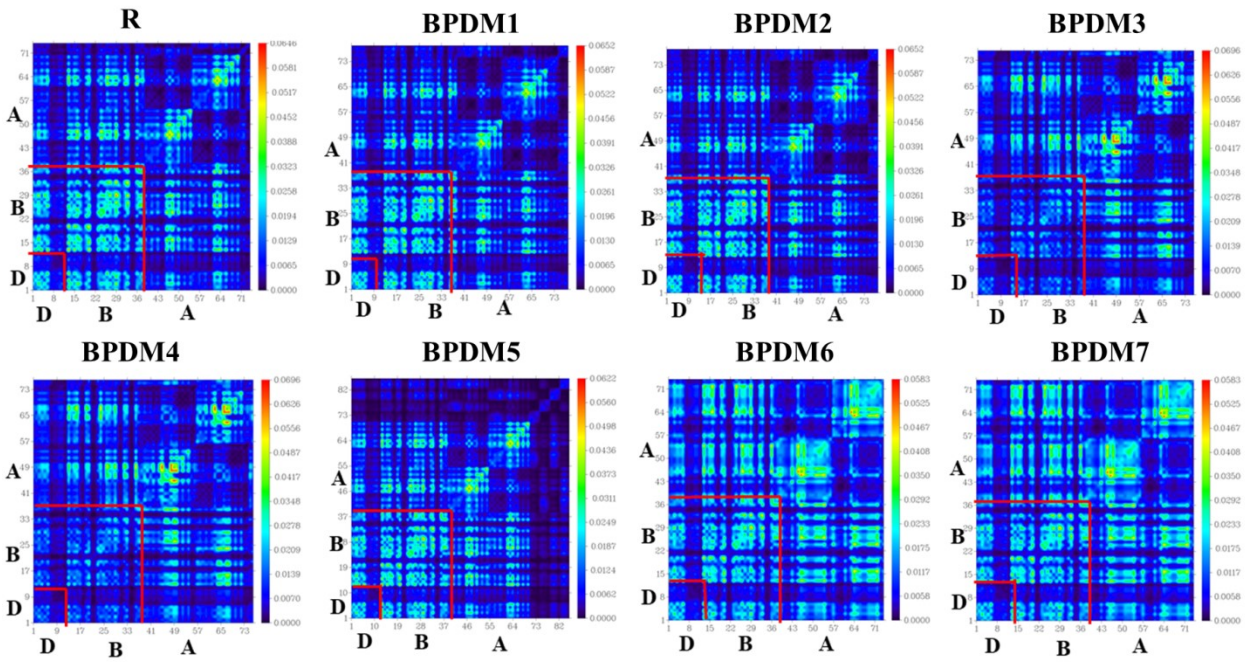

Figure S4 TDM plots of R and designed molecules

Table S1 Calculated absorption profile (λ_{max}), light harvesting efficiency (LHE), Excitation energy (E_X), Oscillating strength (f), and Dipole moments (μ) for R and deigned molecules in gas phase

Molecules	λ_{max} Calculated (nm)	λ_{max} Experimental (nm)	E_X (eV)	Dipole moment (D)	f	LHE	E_b (eV)
R	629	652	1.96	1.82	2.78	0.9992	0.36
BPDM1	642	-	1.93	3.13	3.03	0.9996	0.33
BPDM2	649	-	1.90	0.39	3.04	0.9996	0.34
BPDM3	758	-	1.63	1.62	1.82	0.9924	0.36
BPDM4	752	-	1.64	1.89	1.70	0.9886	0.39
BPDM5	639	-	1.93	1.44	2.89	0.9991	0.38
BPDM6	671	-	1.84	1.52	2.55	0.9982	0.39
BPDM7	640	-	1.93`	3.88	2.81	0.9993	0.34

Table S2 Calculated absorption profile (λ_{max}), light harvesting efficiency (LHE), Excitation energy (E_X), Oscillating strength (f), and Dipole moments (μ) for R and deigned molecules in solvent

Molecules	λ_{max} Calculated (nm)	λ_{max} Experimental (nm)	E_X (eV)	Dipole moment (D)	f	LHE	E_b (eV)
R	670	652	1.84	3.01	3.07	0.9984	0.24
BPDM1	681	-	1.82	2.85	3.37	0.9990	0.22
BPDM2	689	-	1.79	1.21	3.37	0.9991	0.22
BPDM3	829	-	1.49	2.10	2.11	0.9849	0.22
BPDM4	825	-	1.50	2.83	1.94	0.9804	0.24
BPDM5	686	-	1.80	3.45	3.04	0.9987	0.24
BPDM6	737	-	1.68	2.66	2.73	0.9972	0.22
BPDM7	678	-	1.82`	3.62	3.18	0.9985	0.24

Table S3 Theoretically calculated HOMO,LUMO and energy gap (E_g) values of R and designed molecules using the B3LYP/6-31G(d,p) level of theory

Molecules	LUMO (eV)	HOMO (eV)	E_g (eV)
R	-3.46	-5.66	2.20
BPDM1	-3.33	-5.48	2.15
BPDM2	-3.45	-5.58	2.13
BPDM3	-3.51	-5.36	1.85
BPDM4	-3.61	-5.49	1.88
BPDM5	-3.48	-5.66	2.18
BPDM6	-3.61	-5.68	2.07
BPDM7	-3.30	-5.47	2.17

Table S4 Percentage contribution of donors, acceptor and π-bridge in R and designed molecules

Molecules	Excitation energy states	Percentage contribution of donor core (%)	Percentage contribution of acceptor (%)	Percentage contribution of pi-bridge (%)
R	HOMO	10.3	26.5	63.5
	LUMO	9.1	52.8	38.5
BPDM1	HOMO	9.9	28.1	62.5
	LUMO	9.2	53.1	37.7
BPDM2	HOMO	10.2	28.1	61.7
	LUMO	9.0	53.9	37.2
BPDM3	HOMO	9.5	28.7	61.8
	LUMO	3.0	81.4	15.6
BPDM4	HOMO	9.9	28.4	61.7
	LUMO	3.0	80.7	16.2
BPDM5	HOMO	10.5	26.6	62.9
	LUMO	8.9	54.2	37.0
BPDM6	HOMO	10.3	27.0	62.7
	LUMO	6.5	63.3	30.3
BPDM7	HOMO	9.7	29.5	60.8
	LUMO	9.6	51.9	38.5

Table S5 Ionization potential (IP), electron affinity (EA), chemical hardness (η), and global softness (S) for the R and designed molecules (BPDM1–BPDM7) calculated at the B3LYP/6-31G(d,p) level

Molecules	**IP (eV)**	**EA (eV)**	η **(eV)**	**S (eV)**
R	5.66	3.46	1.10	0.450
BPDM1	5.48	3.33	1.075	0.465
BPDM2	5.58	3.45	1.065	0.469
BPDM3	5.36	3.51	0.925	0.541
BPDM4	5.49	3.61	0.94	0.532
BPDM5	5.66	3.48	1.09	0.459
BPDM6	5.68	3.61	1.035	0.483
BPDM7	5.47	3.30	1.085	0.461

Table S6 The reorganization energies of holes (λ_h) and electrons (λ_e) for the R and designed molecules (BPDM1–BPDM7)

Molecules	λ_e **(eV)**	λ_h **(eV)**
R	0.007425	0.007731
BPDM1	0.006702	0.103544
BPDM2	0.016091	0.015454
BPDM3	0.004301	0.006650
BDPM4	0.004053	0.006267
BDPM5	0.007098	0.458086
BPDM6	0.105526	0.463267
BPDM7	0.007235	0.228532

Table S7 Calculated fill factor (FF), open-circuit voltage (V_{oc}), and PCE for the R and the designed molecules (BPDM1–BPDM7)

Molecules	**Fill factor (FF)**	**V_{oc}**	**PCE**
R	92.43%	1.76	25.85%
BPDM1	92.82%	1.88	27.83%
BPDM2	92.43%	1.76	25.85%
BPDM3	92.22%	1.70	24.75%
BPDM4	91.87%	1.61	23.29%
BPMD5	92.36%	1.74	25.54%
BPDM6	91.87%	1.61	23.29%
BPDM7	92.96%	1.93	28.72%