"Theoretical Investigation of Benzodithiophene-Based Donor Molecules in Organic Solar Cells: From Structural Optimization to Performance Metrics"

Syed Muhammad Kazim Abbas Naqvi,[a,b,c] Faheem Abbas,[d] Sadaf Bibi,[e] Muhammad Kamran Shehzad,[f] Norah Alhokbany,[g] Yanan Zhu,[a,b] Hui Long,[a,h] Roman B. Vasiliev,[h] Zahid Nazir *[a] and Shuai Chang *[a,b]

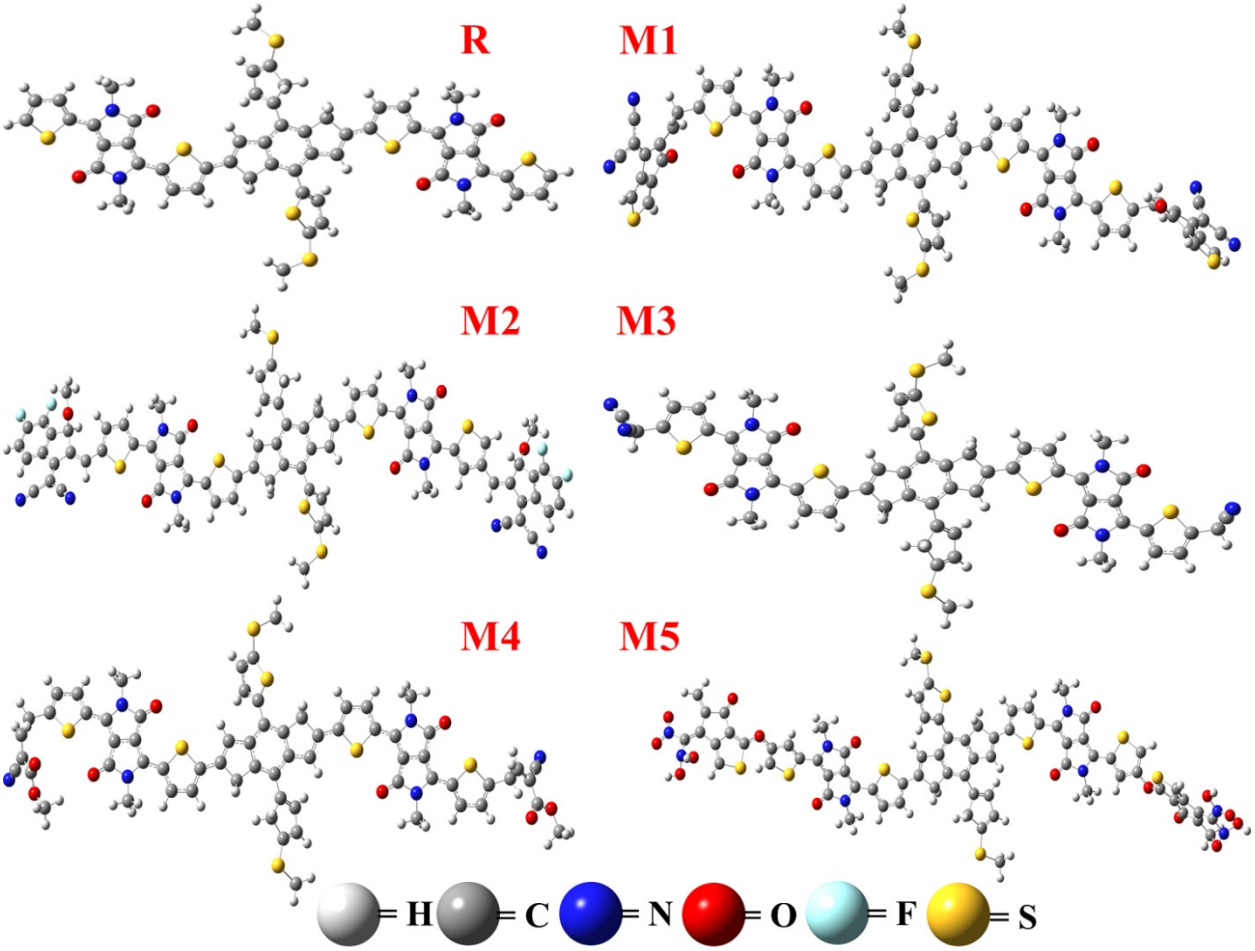

Figure S1. The representation of optimized geometry of Reference molecule R and designed molecules (M1-M5) using MPW1PW91/6-31G (d,p) level of theory.

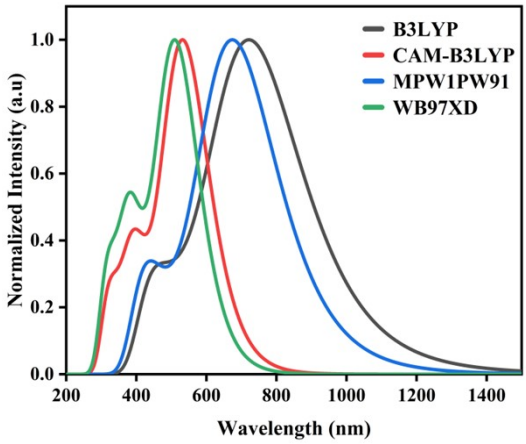

Figure S2. Comparison of four distinct functionals (B3LYP, CAMB3LYP, WB97XD, and MPW1PW91 using MPW1PW91/6-31G (d,p) level of theory.

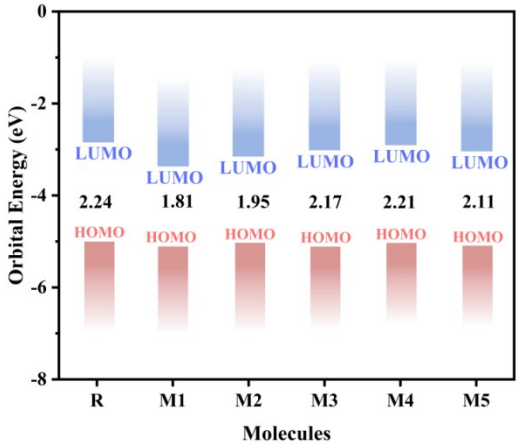

Figure S3. Energy of HOMO, LUMO, and the HOMO-LUMO gap using MPW1PW91/6-31G (d,p) functional for reference molecule R and designed molecules (M1-M5). All the energies are given in electron volts (eV).

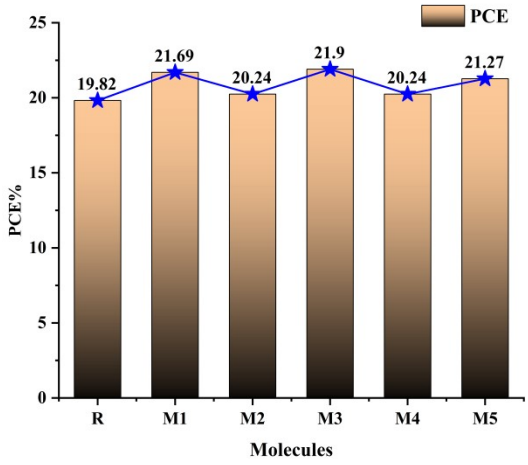

Figure S4. Graphically illustration of power conversion efficiency (PCE%) value of reference molecule R and designed molecules (M1-M5).

Table S1. Calculated absorption profile (λ_{max}), light harvesting efficiency (LHE), Excitation energy (E_X), Oscillating strength (f), percentage assignments (S_0-S_1) and Dipole moments (μ) for reference molecule R and deigned molecules (M1-M5) in polar solvent (dichloromethane).

Molecules	λ_{max} Calculated (nm)	λ_{max} Experimental (nm)	LHE	E_x (eV)	f	Assignment S_0-S_1 (%)	Dipole moment (μ)
R	683	622	0.993	1.813	2.148	H-L (98%)	3.943
M1	846	----	0.966	1.465	1.881	H-L (97%)	13.625
M2	748	----	0.978	1.656	0.361	H-L (97%)	5.689
M3	710	----	0.982	1.744	2.159	H-L (97%)	9.786
M4	699	----	0.983	1.773	2.339	H-L (97%)	4.228
M5	707	----	0.982	1.753	2.294	H-L (97%)	6.360

Table S2. Calculated absorption profile (λ_{max}), light harvesting efficiency (LHE), Excitation energy (E_X), Oscillating strength (f), percentage assignments (S_0-S_1) and Dipole moments (μ) for reference molecule R and deigned molecules (M1-M5) in gas phase.

Molecules	λ_{max} Calculated (nm)	LHE	E_x (eV)	f	Assignment S_0-S_1 (%)	Dipole moment (μ)
R	650	0.989	1.905	1.982	H-L (69%)	3.143
M1	791	0.985	1.567	1.845	H-L (68%)	10.625
M2	832	0.239	1.489	0.119	H-L (52%)	4.212
M3	677	0.990	1.830	2.023	H-L (69%)	7.723
M4	670	0.991	1.849	2.207	H-L (69%)	4.042
M5	650	0.989	1.905	1.982	H-L (69%)	4.862

Table S3. Values of energy gap[a], first singlet excitation energies [b], exciton binding energies [c] of reference molecule R and designed molecules (M1-M5).

Molecules	[a]$E_{H\text{-}L}$ (eV)	[b]E_{Opt} (eV)	[c]E_b (eV)
R	2.24	1.81	0.43
M1	1.81	1.46	0.35
M2	1.95	1.65	0.30
M3	2.17	1.74	0.43
M4	2.21	1.77	0.44
M5	2.11	1.75	0.36