SUPPORTING INFORMATION

Structure-Property Relationship and Design of Carbazole Naphthalene-based Linear Materials for Organic and Perovskite Photovoltaics

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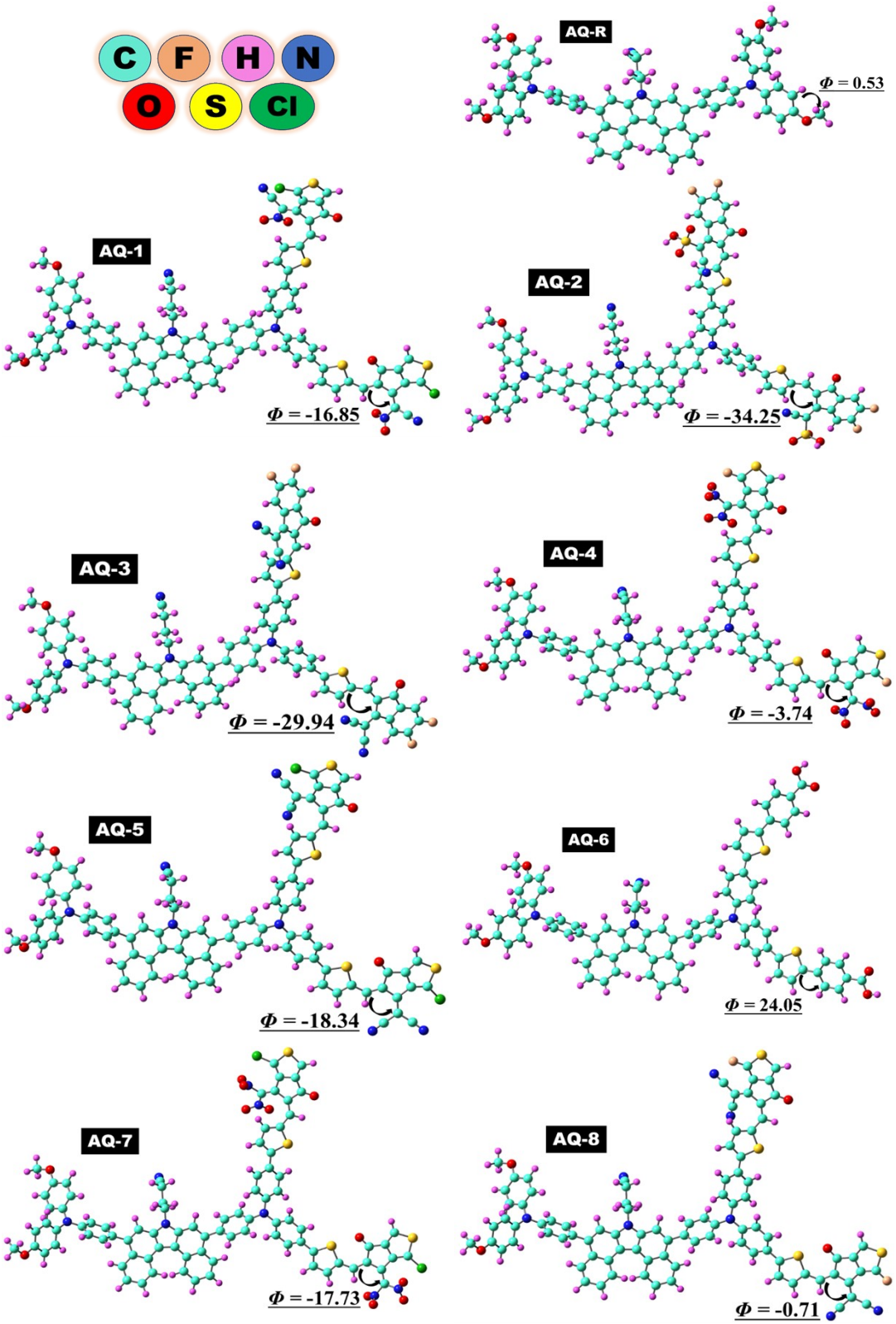

Figure S1. Diagrammatic illustrations of optimized structures of AQ-R and newly designed (AQ-1 to AQ-8) molecules along labelled dihedral angles.

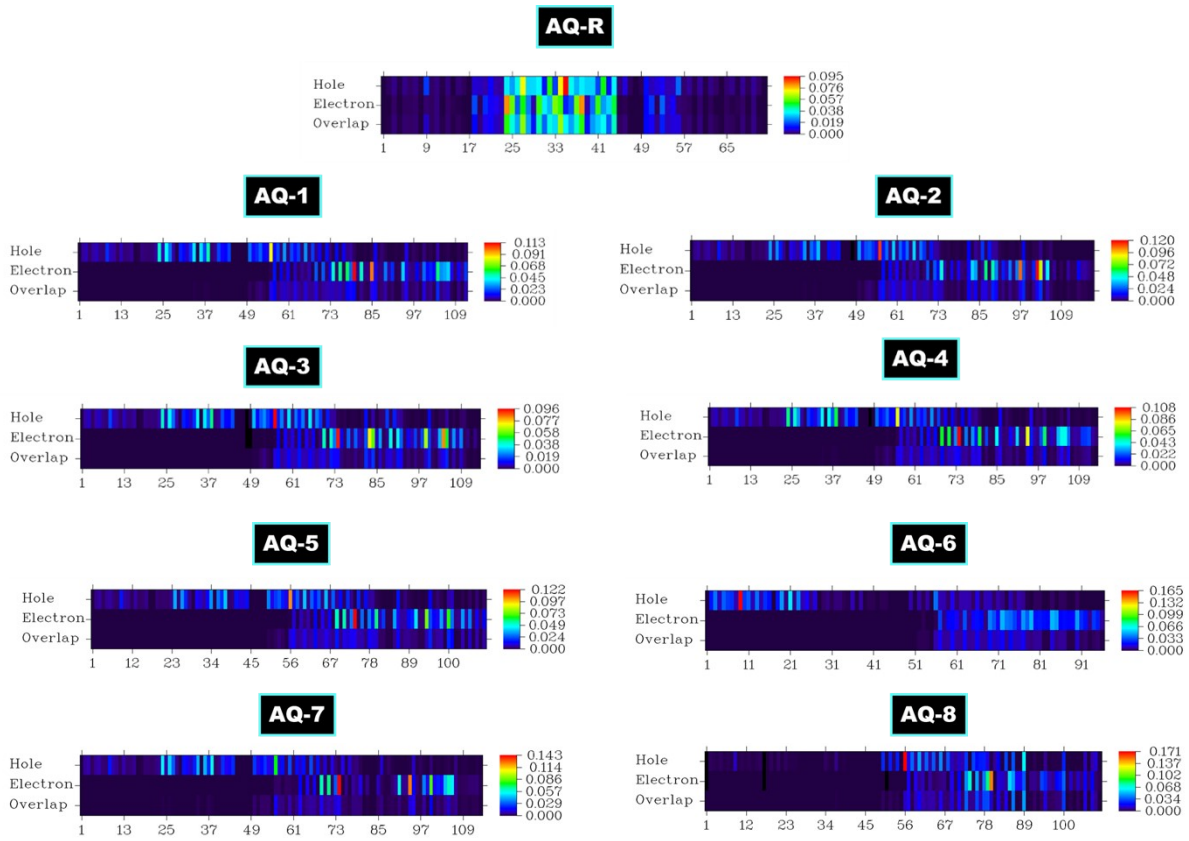

Figure S2. Schematic plots of the Heat map for AQ-R and (AQ-1 to AQ-8) designed molecules.

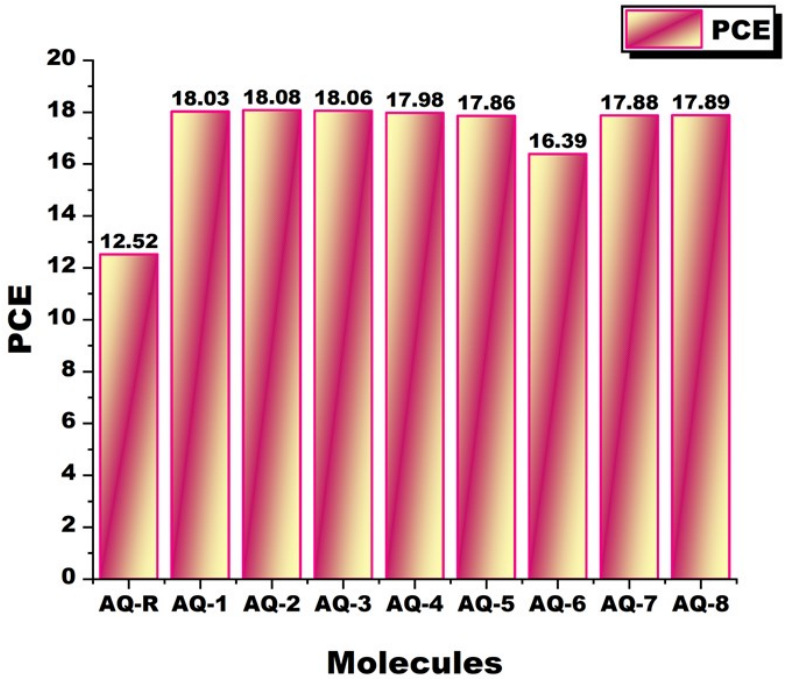

Figure S3. Calculated PCE of AQ-R and newly studied (AQ-1 to AQ-8) molecules.

Table S1: Theoretically evaluated and reported values of λmax of AQ-R at several DFT levels.

DFT Functionals	DFT Computed λ_{max} (nm)	Experimental λ_{max} (nm)
Experimental		401 nm
B3LYP	439.16	
CAMB3LYP	347.66	
M06	419.49	
M062X	356.23	
MPW1PW91	418.51	
***ω*B97XD**	341.24	

Table S2: Computed HOMO-LUMO energies and Eg (L-H) values for synthetic reference AQ-R and designed AQ-1 to AQ-8 molecules.

Molecules	E_{HOMO} (eV)	E_{LUMO} (eV)	$E_g = E_L - E_H$ (eV)
AQ-R	-4.78	-1.20	3.58
AQ-1	-5.02	-3.47	1.55
AQ-2	-5.02	-3.26	1.77
AQ-3	-5.02	-3.34	1.68
AQ-4	-5.02	-3.46	1.56
AQ-5	-5.01	-3.32	1.70
AQ-6	-4.95	-1.86	3.09
AQ-7	-5.01	-3.55	1.46
AQ-8	-5.01	-3.30	1.71

Table S3: Computed and experimentally determined λ_{max}, Excitation energy (E_x), $f_{os,}$ and substantial molecular transformations for (AQ-R) and (AQ-1 to AQ-8) at MPW1PW91/6-31G (d, p) in gas medium.

Molecules	DFT Calculated $\lambda_{max\ (}$nm)	Experimental $\lambda_{max\ (}$nm)	E_x (eV)	f_{os}	Major MO Assignment
AQ-R	408.76	401	3.03	1.26	HOMO > LUMO (95%)
AQ-1	612.84		2.02	0.64	HOMO > LUMO (85%)
AQ-2	635.33		1.95	0.67	H-2->LUMO (14%), H-1->LUMO (83%)
AQ-3	582.82		2.13	0.61	H-2->LUMO (85%), H-1->LUMO (12%)
AQ-4	608.18		2.04	0.63	HOMO > LUMO (89%)
AQ-5	436.40		2.84	0.62	HOMO > LUMO (77%)
AQ-6	424.65		2.92	1.40	H-1->L+1 (22%), HOMO->L+1 (47%), HOMO->L+2 (24%)
AQ-7	638.07		1.94	0.44	HOMO > LUMO (85%)
AQ-8	431.73		2.87	0.64	HOMO > LUMO (81%)

Table S4: Arithmetically measured Dihedral angles of AQ-R and newly studied (AQ-1-AQ-8) compounds.

Molecules	*Dihedral Angle Φ*
AQ-R	0.53
AQ-1	-16.85
AQ-2	-34.25
AQ-3	-29.94
AQ-4	-3.74
AQ-5	-18.34
AQ-6	24.05
AQ-7	-17.73
AQ-8	-0.71

Table S5: Theoretically computed values of Eg (L-H), Eoptimization, and Eb of AQ-R and (AQ-1 to AQ-8) compounds.

Molecules	Eg (L-H) (eV)	Eopt (sol) (eV)	Eb (sol) = Eg - Eopt (eV)
AQ-R	3.58	2.96	0.61
AQ-1	1.55	1.41	0.13
AQ-2	1.77	1.67	0.10
AQ-3	1.68	1.61	0.07
AQ-4	1.56	1.41	0.15
AQ-5	1.70	1.60	0.10
AQ-6	3.09	2.74	0.35
AQ-7	1.46	1.28	0.18
AQ-8	1.71	1.62	0.09

Table S6: Calculated values for $\lambda_{hole,}$ $\lambda_{electron,}$ $T_{(hole),}$ and $T_{(electron)}$ of AQ-R along with (AQ-1-AQ-8) designed structures.

Molecules	λe	λh	$T_{(hole)}$	$T_{(electron)}$
AQ-R	0.0088	0.0032	0.08	0.33
AQ-1	0.0047	0.0040	0.25	0.04
AQ-2	0.0061	0.0040	0.24	0.04
AQ-3	0.0037	0.0040	0.25	0.04
AQ-4	0.0063	0.0040	0.26	0.05
AQ-5	0.0030	0.0038	0.24	0.05
AQ-6	0.0057	0.0028	0.13	0.06
AQ-7	0.0071	0.0040	0.25	0.07
AQ-8	0.0032	0.0038	0.25	0.05

Table S7: Computed values of V_{oc}, %FF, and PCE of model AQ-R and (AQ-1 to AQ-8) compounds.

Molecules	Voc	FF%	PCE
AQ-R	0.58	89.67%	12.52
AQ-1	0.82	91.07%	18.03
AQ-2	0.82	91.08%	18.08
AQ-3	0.82	91.08%	18.06
AQ-4	0.82	91.06%	17.98
AQ-5	0.81	91.04%	17.86
AQ-6	0.75	90.70%	16.39
AQ-7	0.81	91.04%	17.88
AQ-8	0.81	91.04%	17.89