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Boosting the photoelectric conversion efficiency of DSSCs through graphene quantum dots: Insights from theoretical study

Yuanchao Li [a], Wenyuan Zhang [a], Xin Li* [a], Yanling Xu[b]

* Corresponding authors

a. MIIT Key Laboratory of Critical Materials Technology for New Energy Conversion and Storage, School of Chemistry and Chemical Engineering, State Key Lab of Urban Water Resource and Environment, Harbin Institute of Technology, Harbin 150090, China

E-mail: lixin@hit.edu.cn Tel:+86-0451-86282153

b. School of Chemistry and Chemical Engineering, Harbin Institute of Technology, Harbin 150090, China

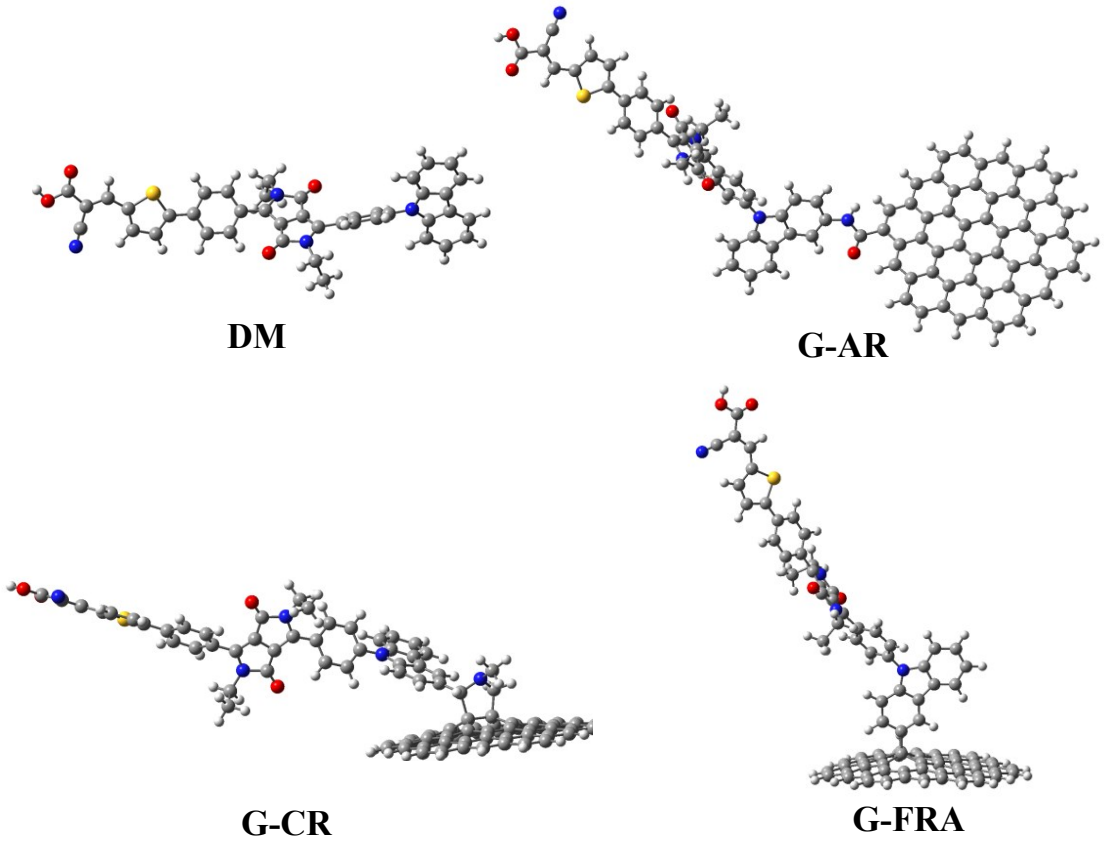

Fig. S1. Optimized ground state structures of nanocomposites and DM.

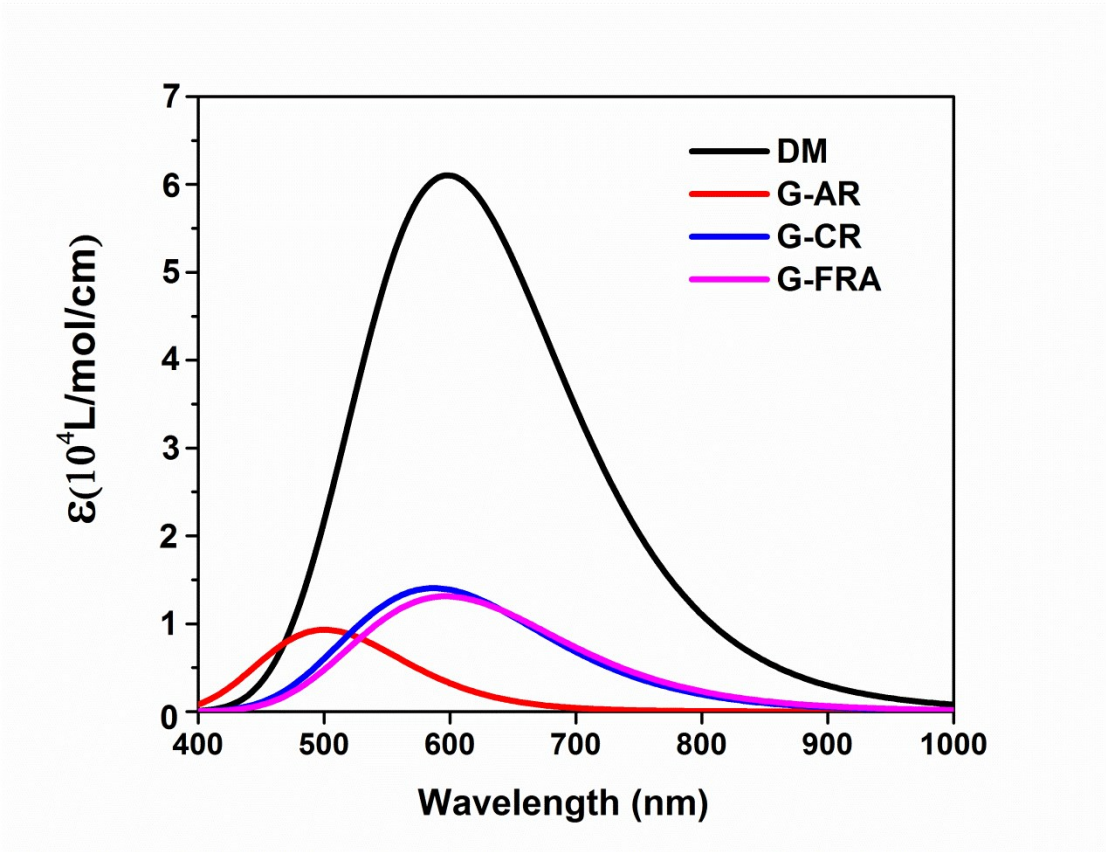

Fig. S2. Simulated fluorescence spectra of DM and nanocomposites. Note that the values of the G-AR are enlarged by 100 times to increase the visibility.

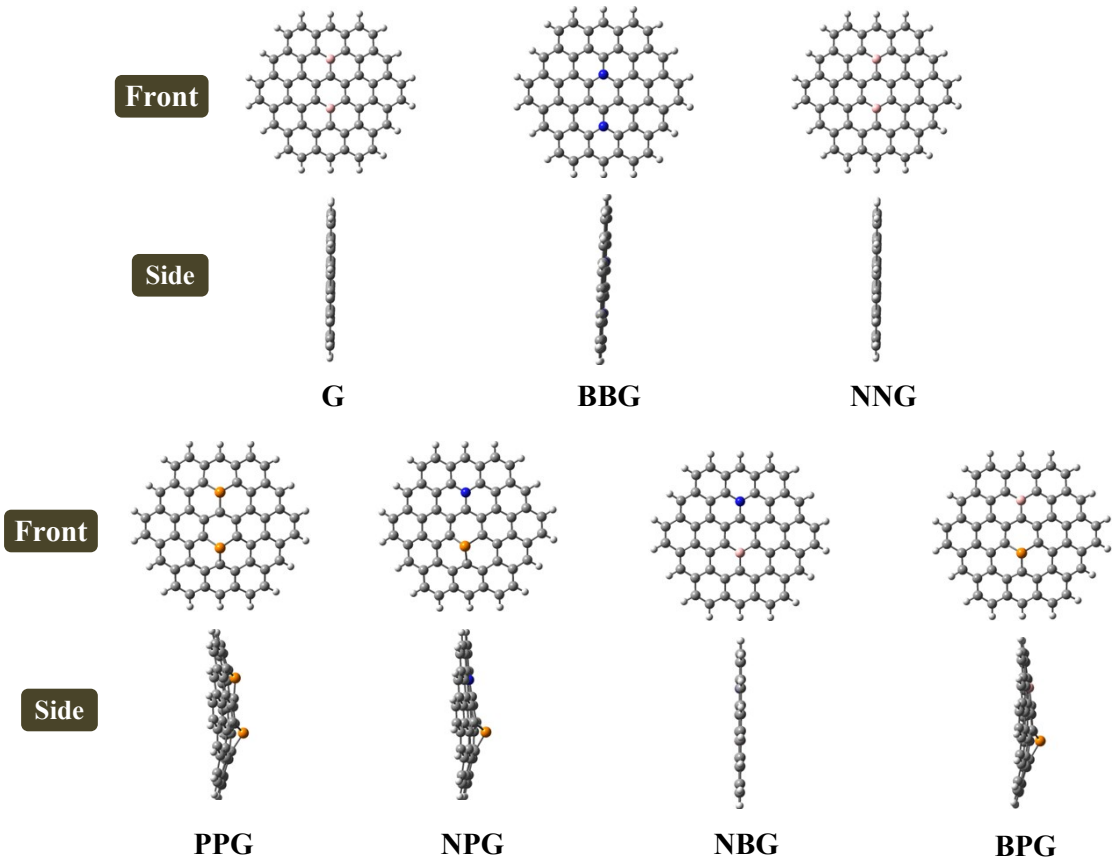

Fig. S3. Optimized structures of pristine and doped GQD in front and side view.

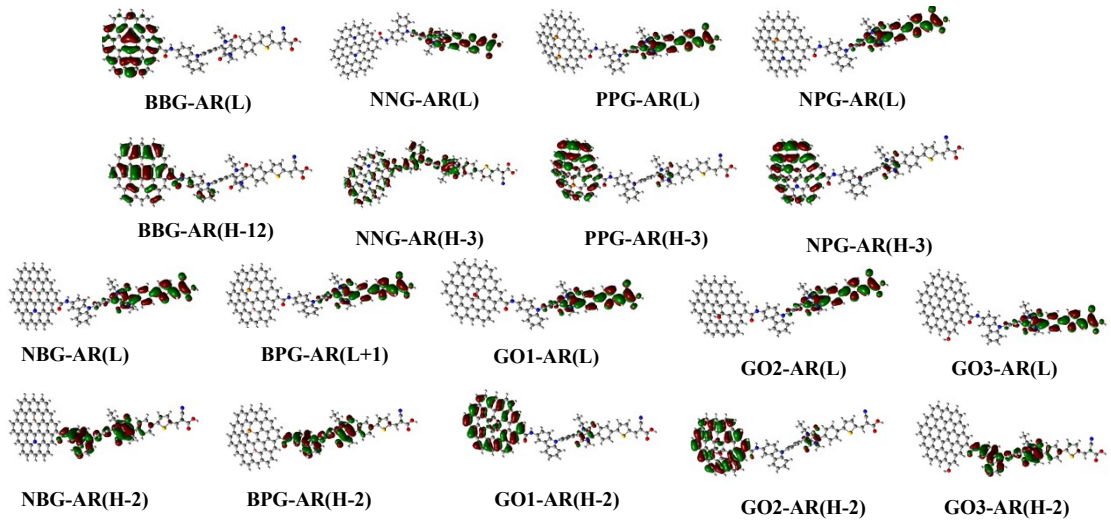

Fig. S4. The selected frontier molecular orbitals (FMOs) of nanocomposites.

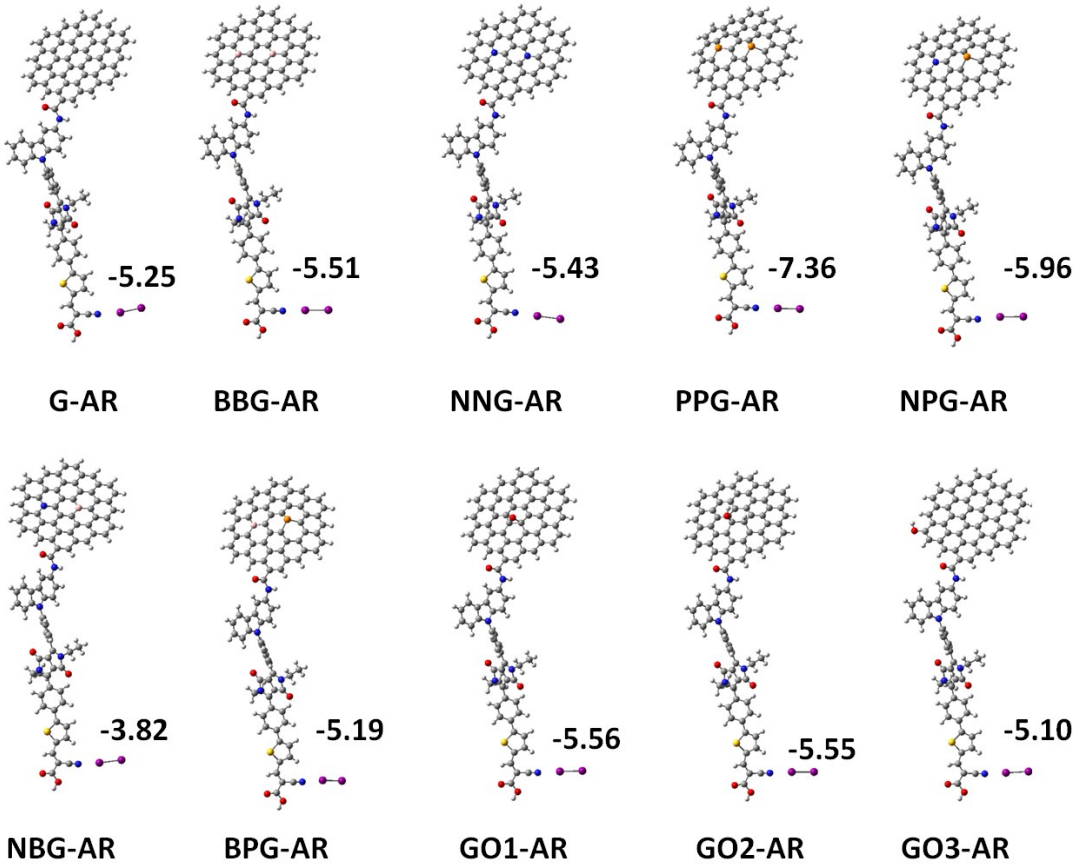

Fig. S5. The binding energies of the nanocomposites-I_2 complex (unit in kcal mol^{-1}).

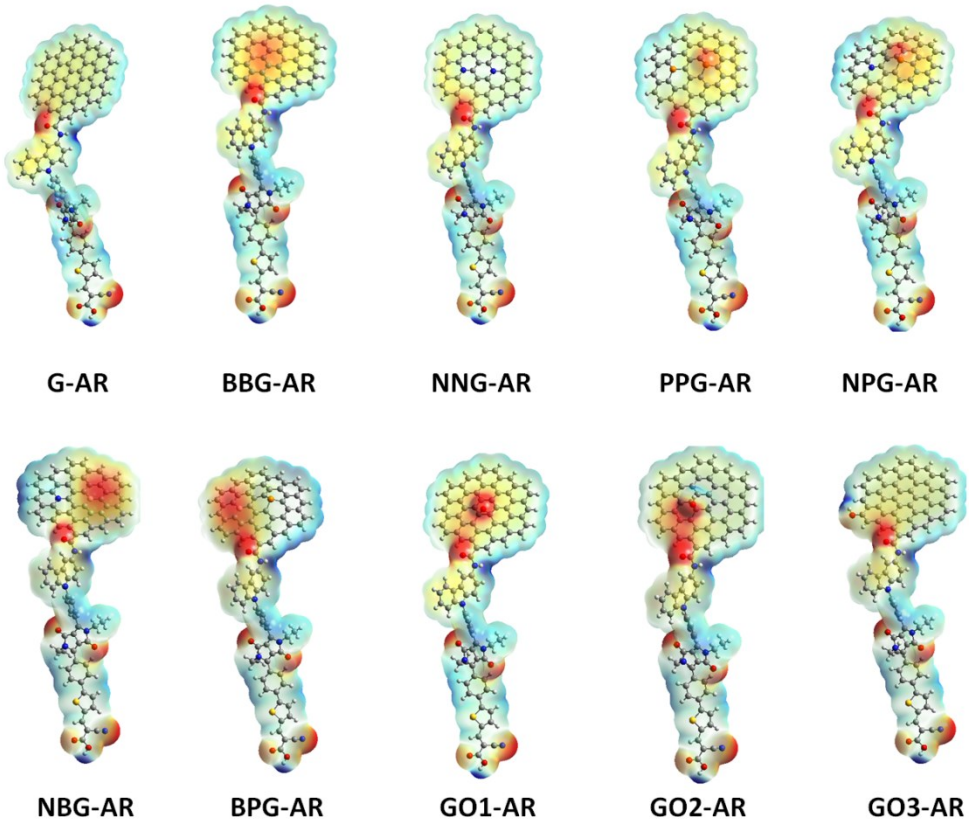

Fig. S6. The molecular electrostatic potential (MEP) of the nanocomposites.

Table S1 The effects of functional on the absorption peaks (nm) of dye DM.

B3LYP	CAM-B3LYP	M062X	MPW1PW91	B3PW91	Exp
594	461	467	555	593	455

Table S2 The calculated bond lengths (Å) and dihedral angles (°) of dye DM and nanocomposites.

	DM	G-AR	G-CR	G-FRA
Φ_1	-52.38	-51.22	-52.40	-51.64
Φ_2	-37.90	-38.34	-39.98	-38.98
Φ_3	-37.90	-37.11	-37.94	-37.81
Φ_4	-20.46	-20.21	-20.49	-20.20
Φ_5	-179.40	-179.28	-179.54	-179.42
d_1	1.417	1.416	1.417	1.417
d_2	1.465	1.465	1.465	1.465
d_3	1.464	1.464	1.464	1.464
d_4	1.463	1.463	1.463	1.463
d_5	1.425	1.425	1.425	1.425

Table S3 Energy level and energy gap (in eV) of dye DM and nanocomposites.

	DM	G-AR	G-CR	G-FRA
LUMO+2	-1.21	-2.35	-2.40	-2.44
LUMO+1	-2.45	-2.45	-2.44	-2.46
LUMO	-2.99	-3.00	-2.99	-2.99
HOMO	-5.36	-5.13	-4.85	-4.88
HOMO-1	-5.70	-5.15	-5.20	-5.29
HOMO-2	-5.99	-5.31	-5.35	-5.37
HL gap	2.37	2.13	1.86	1.89

Table S4 Calculated fluorescence properties of dye DM and nanocomposites.

	State	E_{flu} (eV)	λ_{flu} (nm)	f_{flu}	Transitions
DM	S1	2.07	598	1.5072	H→L/87.14%
G-AR	S1	2.48	500	0.0023	H→L+1/40.03%
G-CR	S1	2.08	597	0.3239	H→L+1/93.72%
G-FRA	S1	2.11	587	0.3468	H→L+1/93.54%

Table S5 The absorption characteristics of nanocomposites.

Dye	E(eV)	λ_{max} (nm)	f	Main configuration
BBG-AR	2.67	464	0.8864	H-12→L/21.75%
NNG-AR	2.68	463	1.6095	H-3→L/47.34%
PPG-AR	2.68	462	1.4633	H-3→L/39.94%
	3.54	351	0.9703	H-6→L+1/35.12%
NPG-AR	2.68	462	1.4744	H-3→L/41.24%
	3.36	369	1.3315	H→L+11/29.44%
NBG-AR	2.68	463	1.6611	H-2→L/46.60%
	3.12	397	1.2457	H-1→L+2/56.90%
	3.28	378	0.9944	H-7→L+1/32.65%
	3.40	365	0.8723	H-4→L+2/36.85%
BPG-AR	2.68	462	1.5183	H-2→L+1/49.41%
	3.35	370	0.9128	H-1→L+4/30.22%
GO1-AR	2.68	462	1.4838	H-2→L/44.18%
	3.13	396	1.0722	H→L+3/40.83%
	3.49	356	0.9450	H-1→L+3/46.36%
GO2-AR	2.68	462	1.4850	H-2→L/42.92%
GO3-AR	2.68	463	1.4949	H-2→L/50.12%
	3.25	382	2.2130	H-1→L+2/38.58%
	3.27	379	1.6914	H-1→L+1/37.27%
	3.28	378	1.0657	H-8→L/52.88%