

Supplementary Materials

Theoretical study on molecular design and optical properties of organic sensitizers

Nachimuthu Santhanamoorthi, Kuan-Hwa Lai, Fadlilatul Taufany and Jyh-Chiang Jiang*

Department of Chemical Engineering, National Taiwan University of Science and Technology,
Taipei-106, Taiwan.

* Corresponding author

E-mail: jcjiang@mail.ntust.edu.tw, Telephone: +886-2-27376653. Fax: +886-2-27376644.

Table 1S. The calculated maximum absorption wavelength (in nm) for P1B, P2B and TC1 dyes using different DFT functionals at 6-31G* level.

Dyes	Medium	B3LYP	CAM-B3LYP	BH and HLYP	M062X	M06HF	wB97XD	ZINDO	Exp^a
P1B	Gas	431	354	352	358	319	346	373	-
	THF	454	366	366	371	327	357	388	385
	Methanol	454	365	364	370		356	386	-
P2B	Gas	337	297	290	299	278	294	335	-
	THF	352	307	299	310	286	303	346	329
	Methanol	353	307	299	310	286	304	346	-
TC1	Gas	418	359	353	363	331	354	388	-
	THF	451	382	374	387	349	375	416	-
	Methanol	451	382	374	387	349	375	415	400

^a. Taken from Ref. [41] and [42]

Table 2S. The calculated maximum absorption wavelength (in nm) for D- $[\pi]_n$ -A₁ series of sensitizers using ZINDO and M06-2X/6-31G* methods.

Sensitizer	State	ZINDO	M06-2X
D- $[\pi]_1$ -A ₁	S ₀ → S ₁	364	328
D- $[\pi]_2$ -A ₁	S ₀ → S ₁	368	333
D- $[\pi]_3$ -A ₁	S ₀ → S ₁	371	337
D- $[\pi]_4$ -A ₁	S ₀ → S ₁	372	339

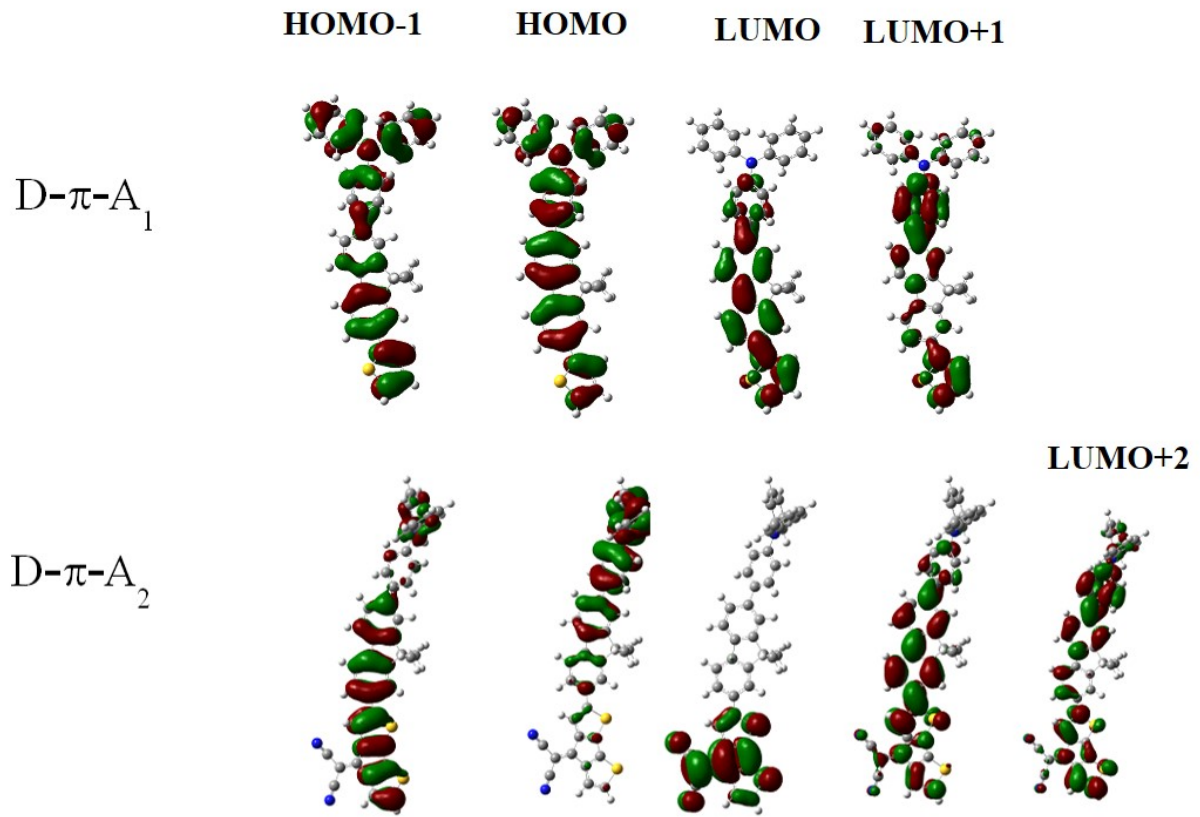


Figure 1S. Selected isodensity plots of the frontier MOs for D- π -A₁ and D- π -A₂ sensitizers

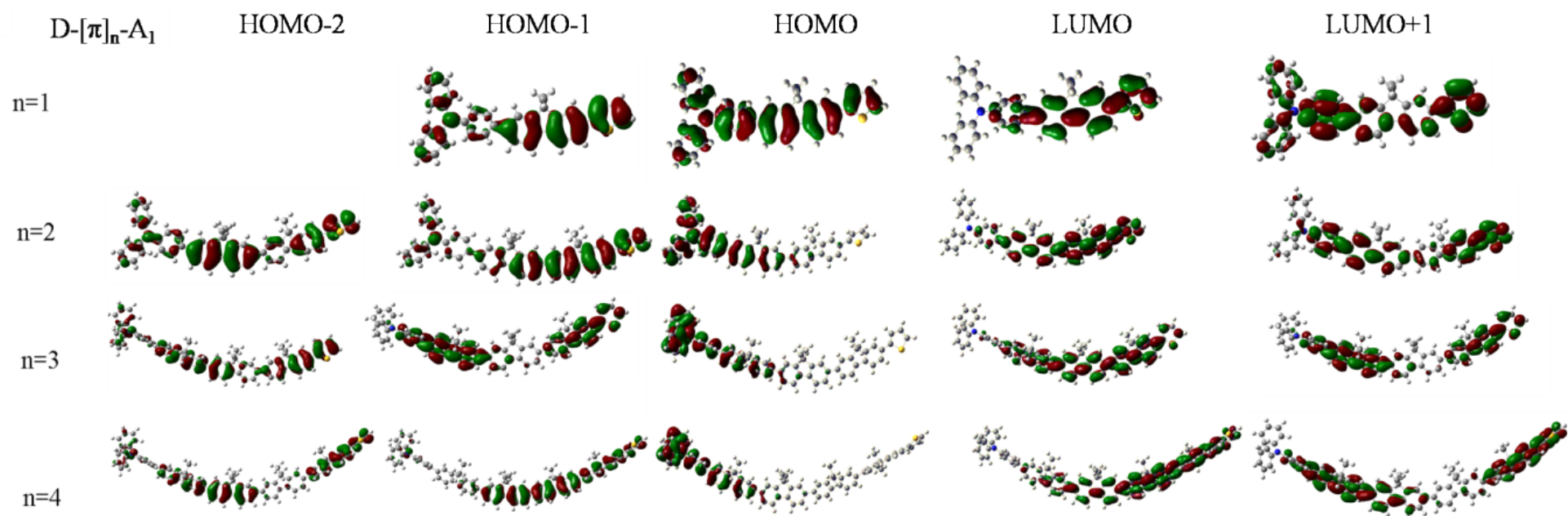


Figure 2S. Selected isodensity plots of the frontier MOs for D- $[\pi]_n$ -A₁ series sensitizers.

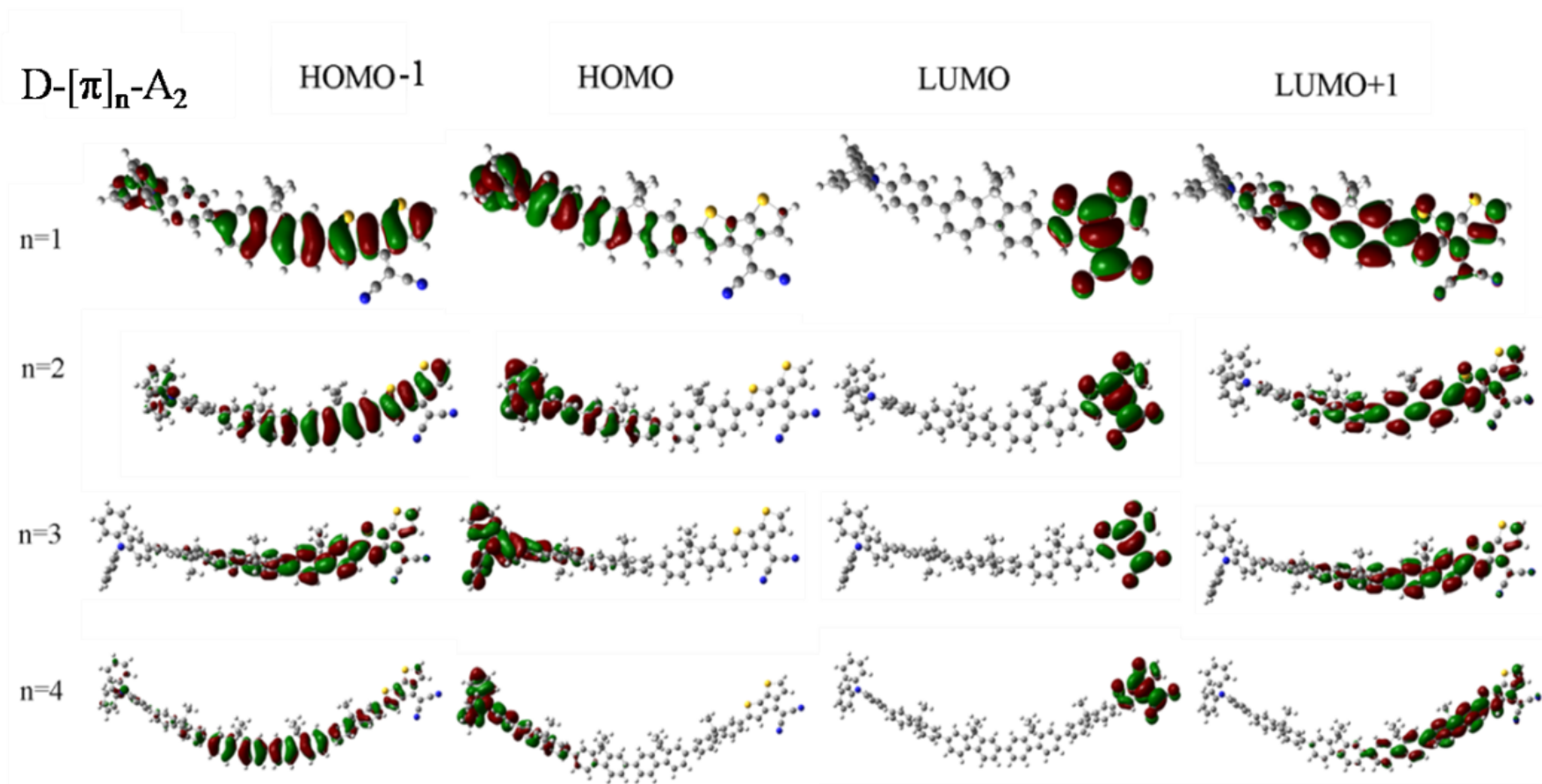


Figure 3S. Selected isodensity plots of the frontier MOs for $D-[\pi]_n-A_2$ series sensitizers.

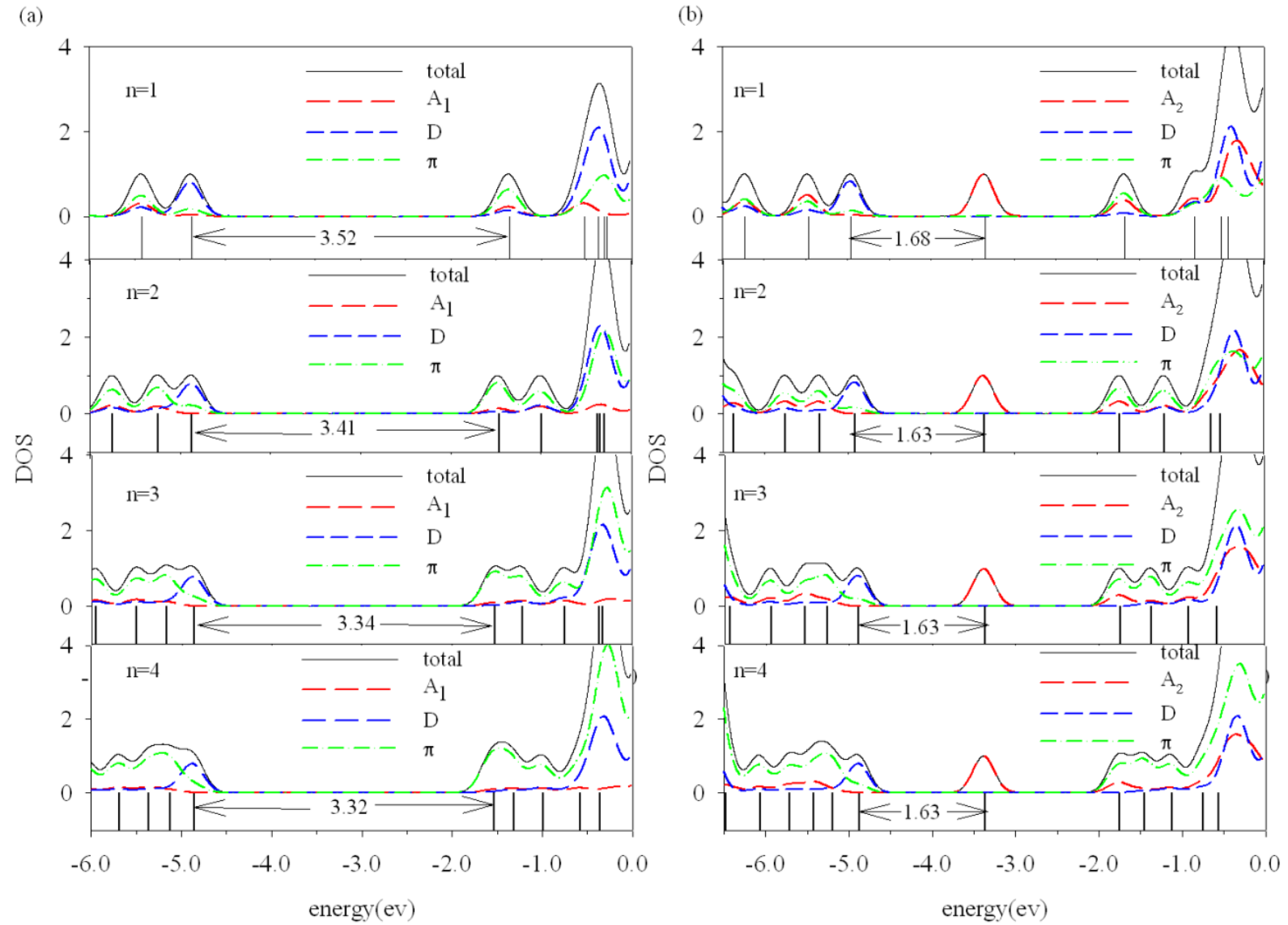


Figure 4S. The total density of states of (a) D-[π]_n-A₁ (b) D-[π]_n-A₂ sensitizers

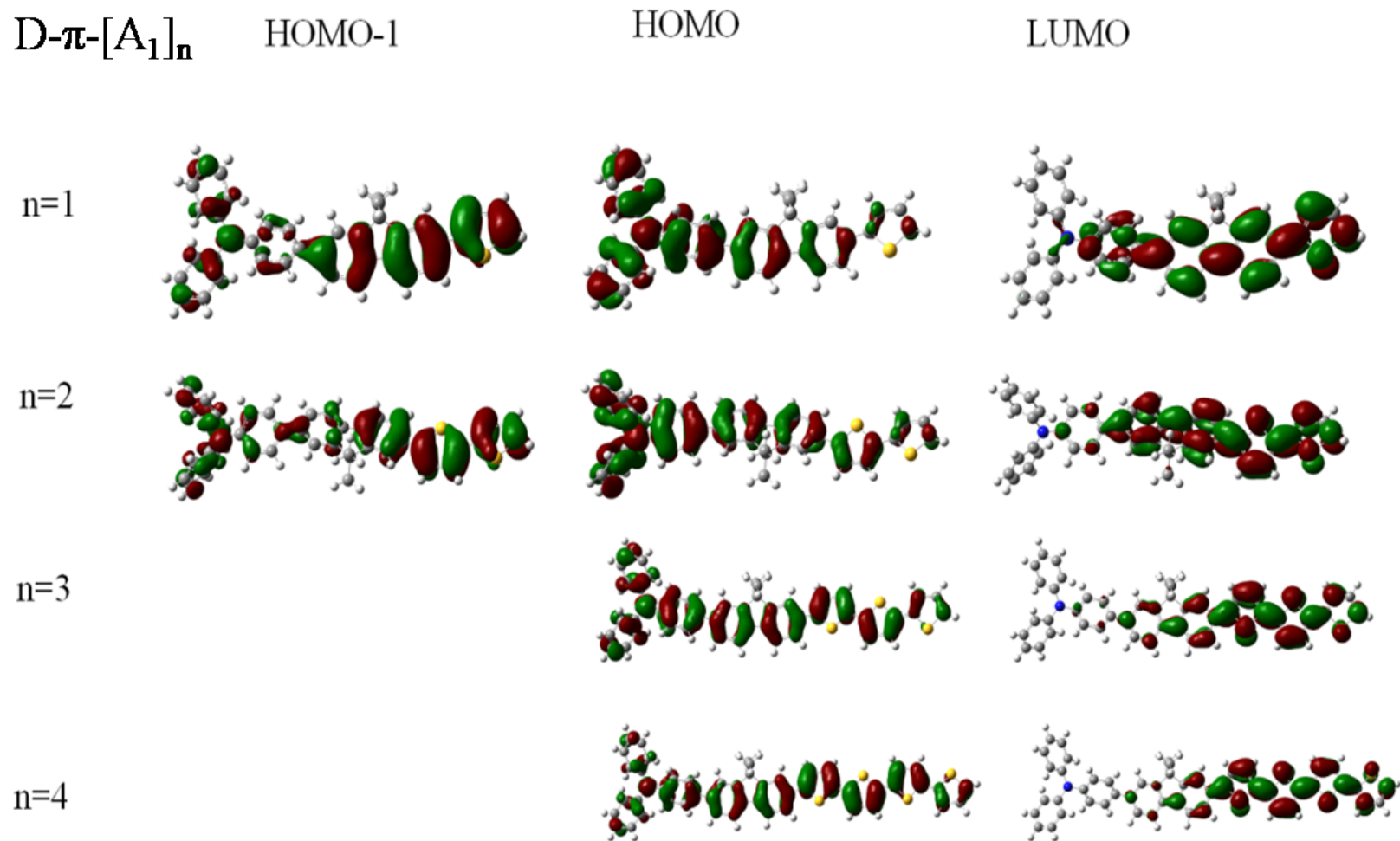


Figure 5S. Selected isodensity plots of the frontier MOs for $D-\pi-[A_1]_n$ series sensitizers

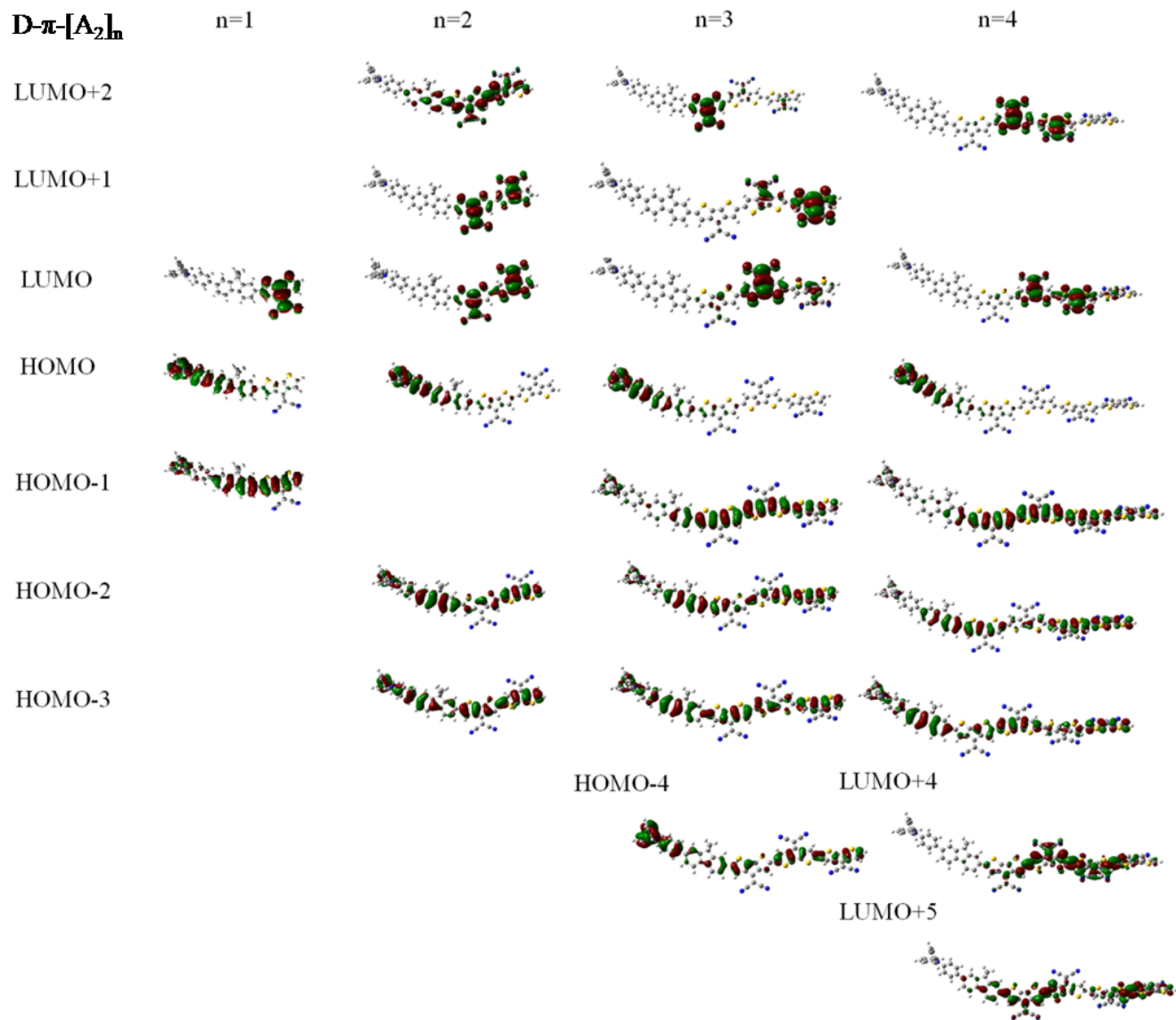


Figure 6S. Selected isodensity plots of the frontier MOs for $D-\pi-[A_2]_n$ series sensitizers

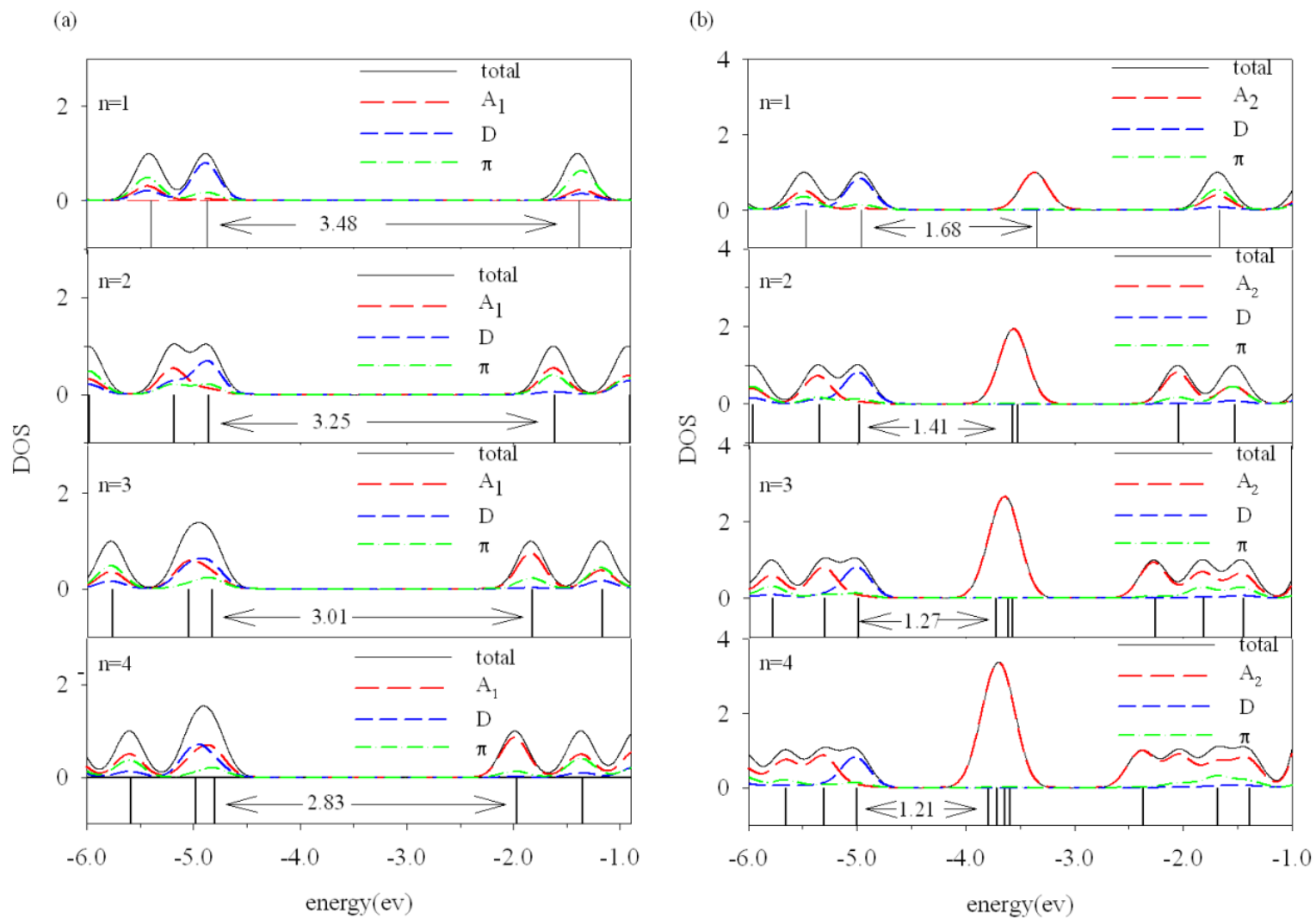


Figure 7S. The total density of states of (a) $D-\pi-[A_1]_n$ (b) $D-\pi-[A_2]_n$ sensitizers

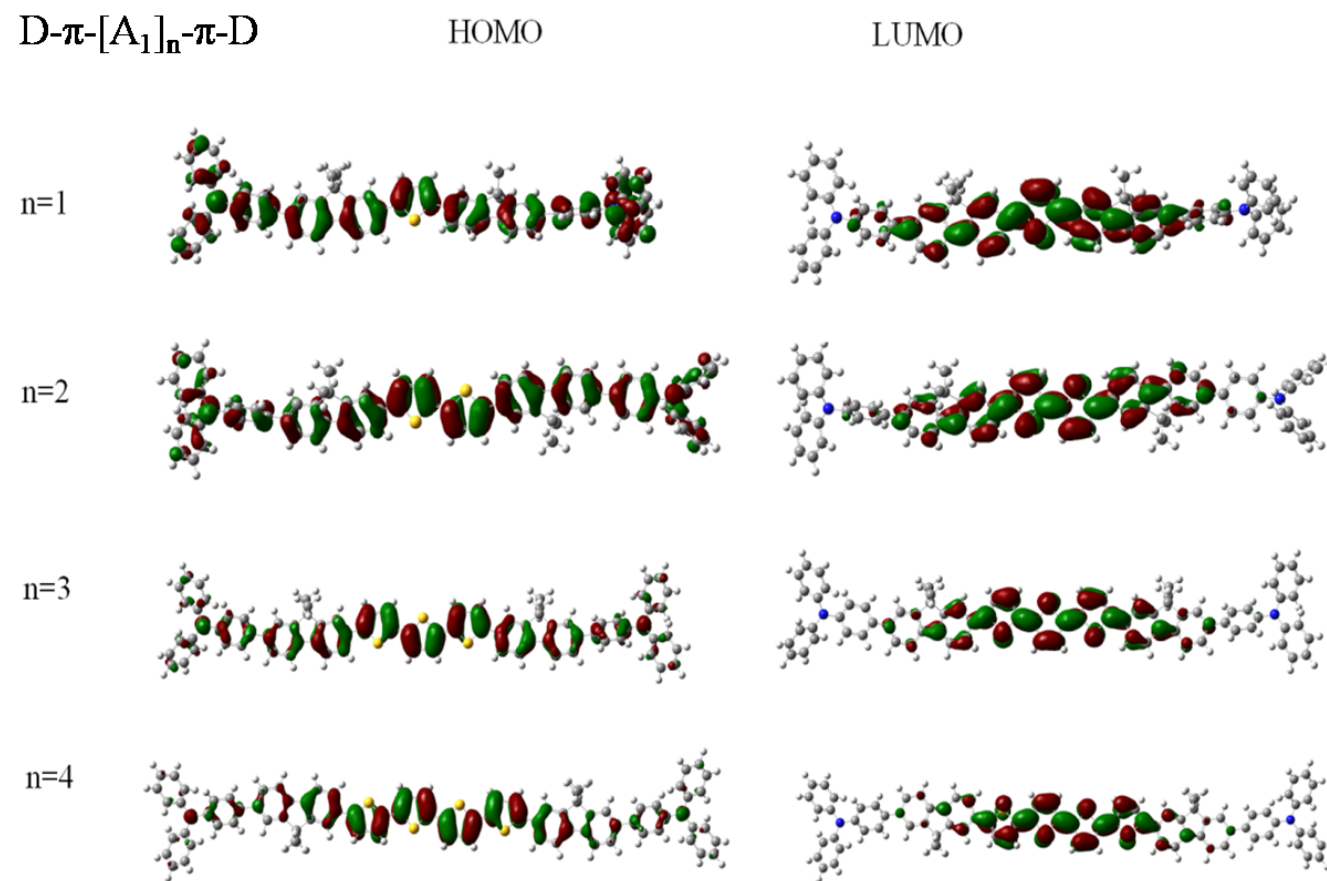


Figure 8S. Selected isodensity plots of the frontier MOs for D- π -[A₁]_n- π -D series sensitizers

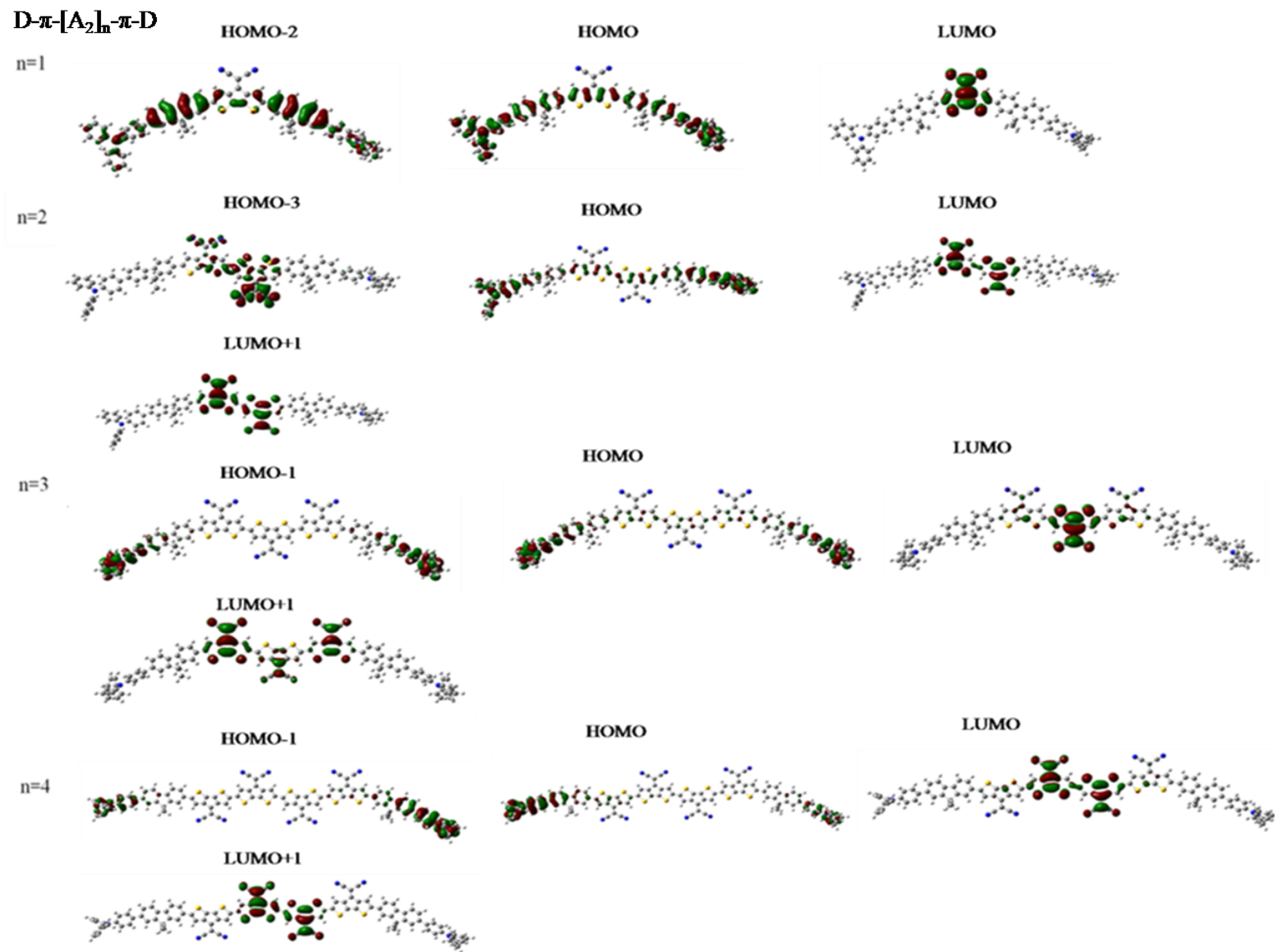


Figure 9S. Selected isodensity plots of the frontier MOs for $D-\pi-[A_2]_n-\pi-D$ series sensitizers

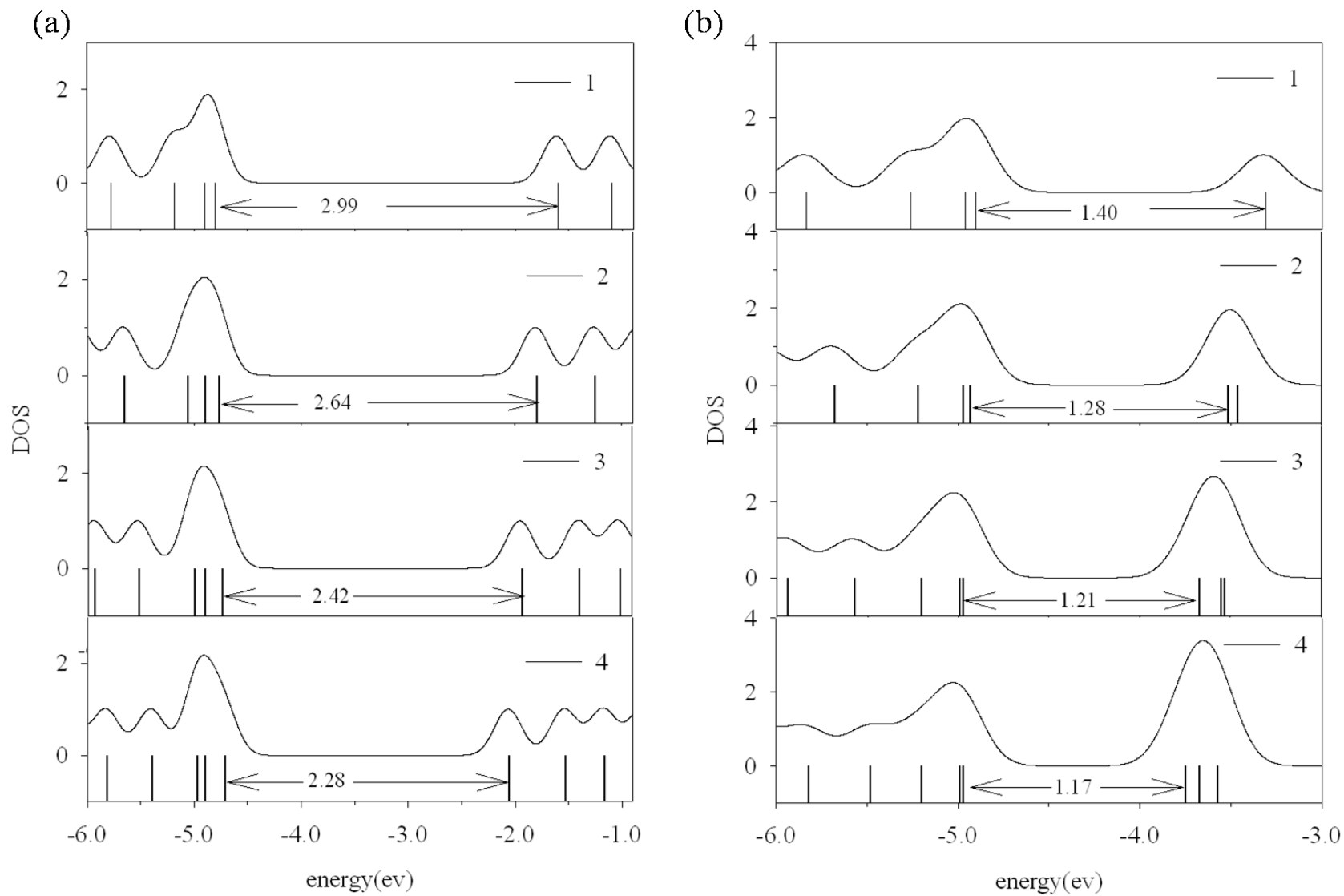


Figure 10S. The total density of states of (a) D- π -[A₁]_n- π -D (b) D- π -[A₂]_n- π -D sensitizers

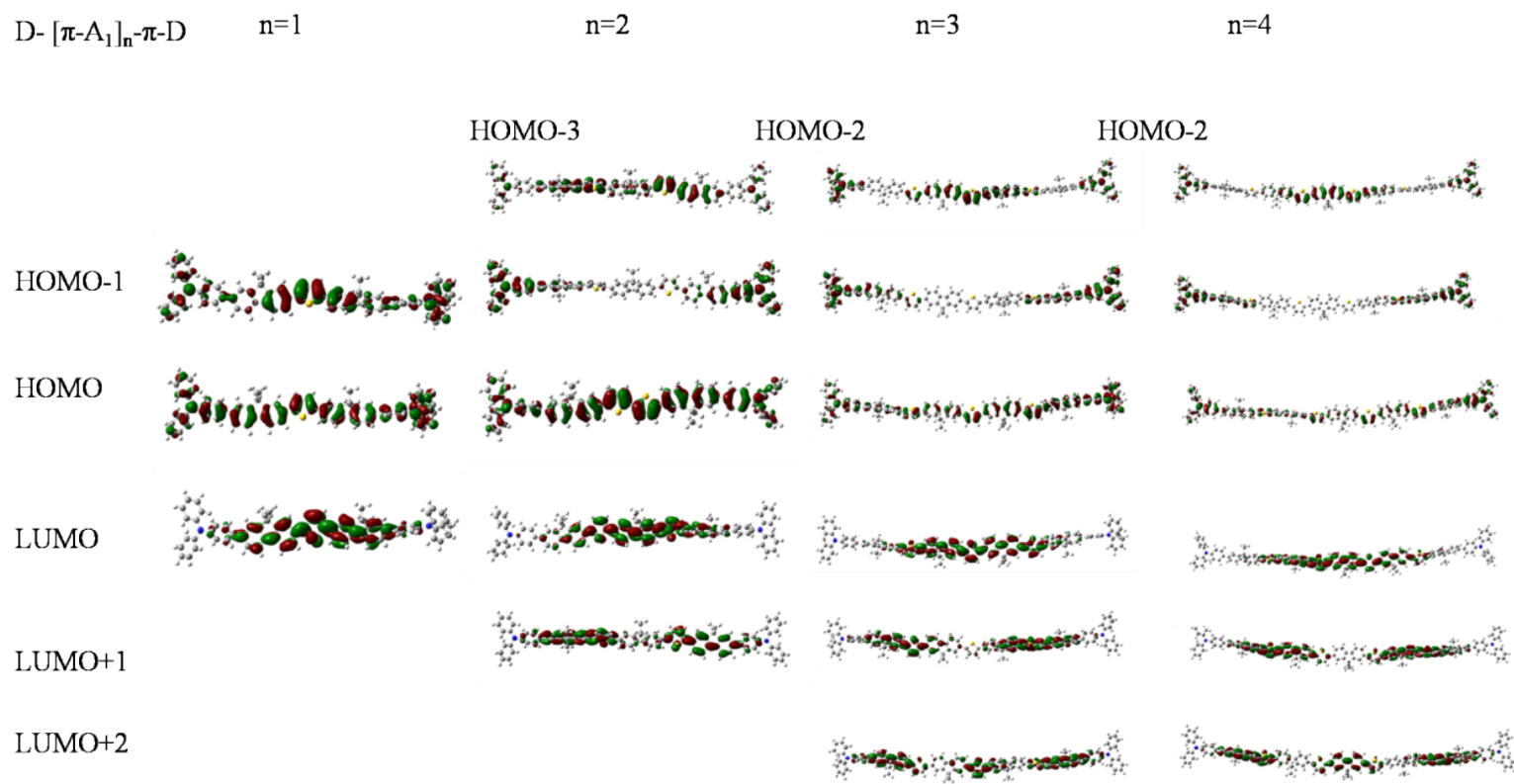


Figure 11S. Selected isodensity plots of the frontier MOs for D- $[\pi-A_1]_n$ - π -D series sensitizers

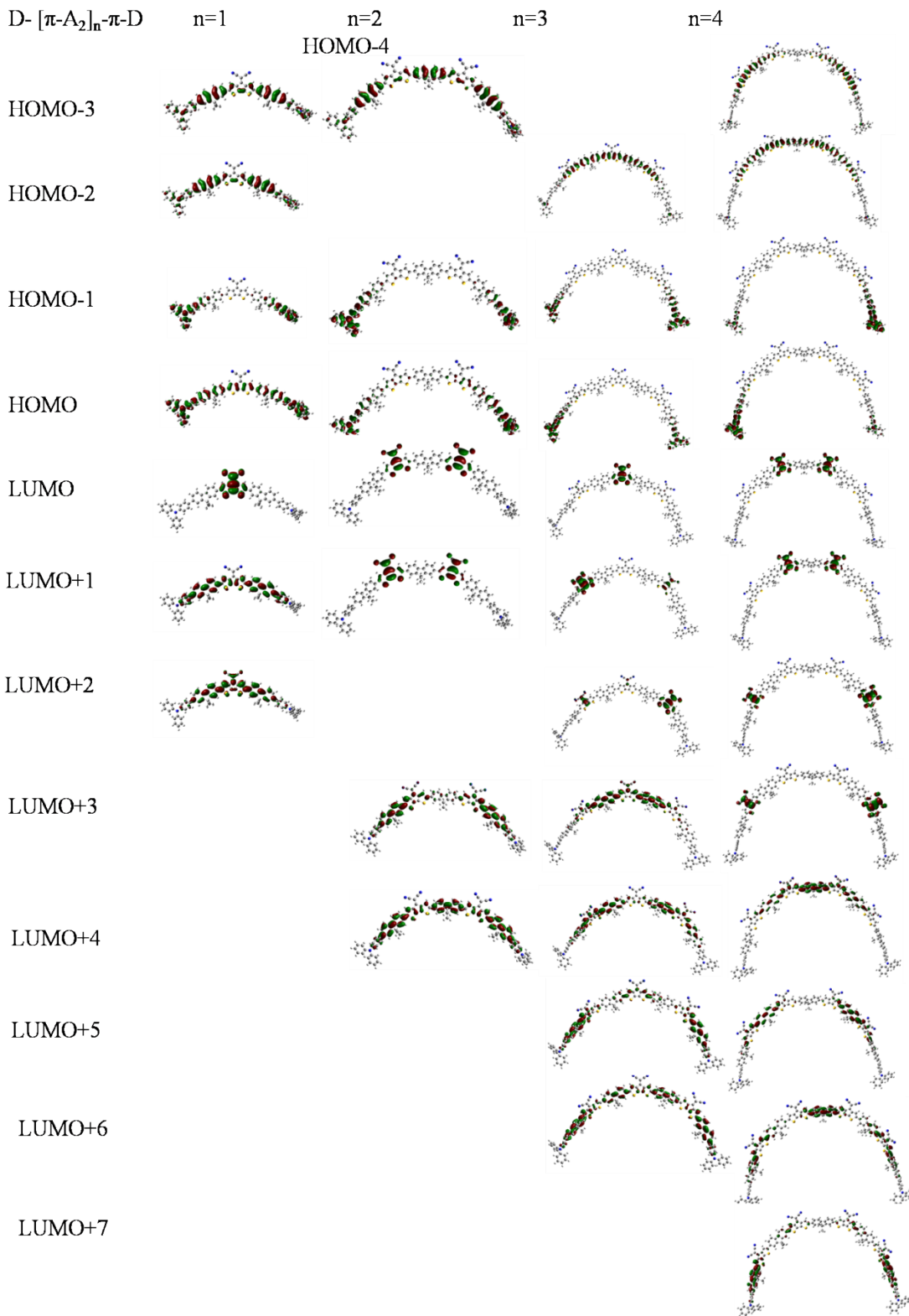


Figure 12S. Selected isodensity plots of the frontier MOs for D- $[\pi-A_2]_n$ - π -D series sensitizers