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Theoretical insights into the effect of pristine, doped and hole graphene on the overall performance of dye-sensitized solar cells

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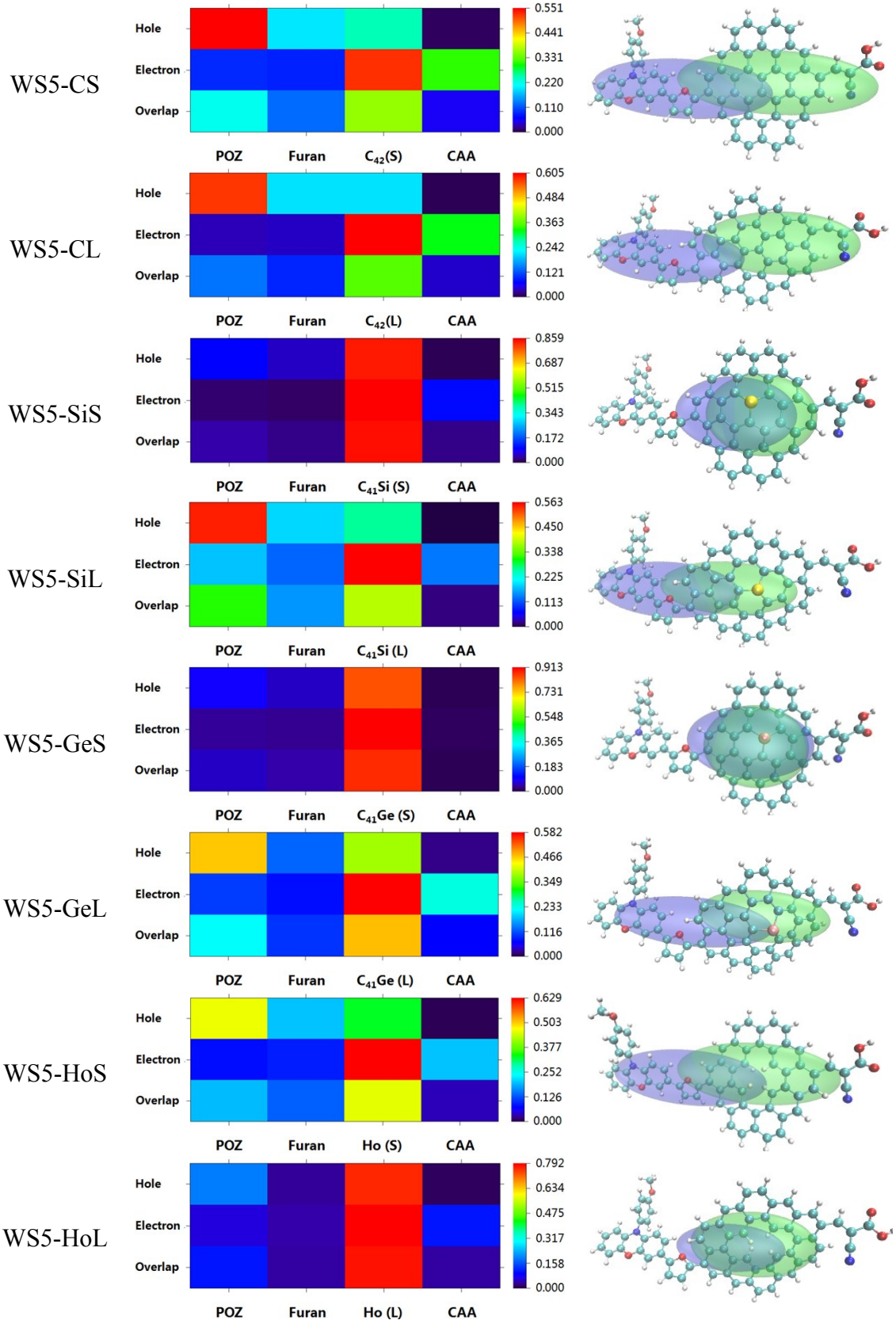

Figure S1 The heat map (left) and centroids of charge (right) of all designed dyes.

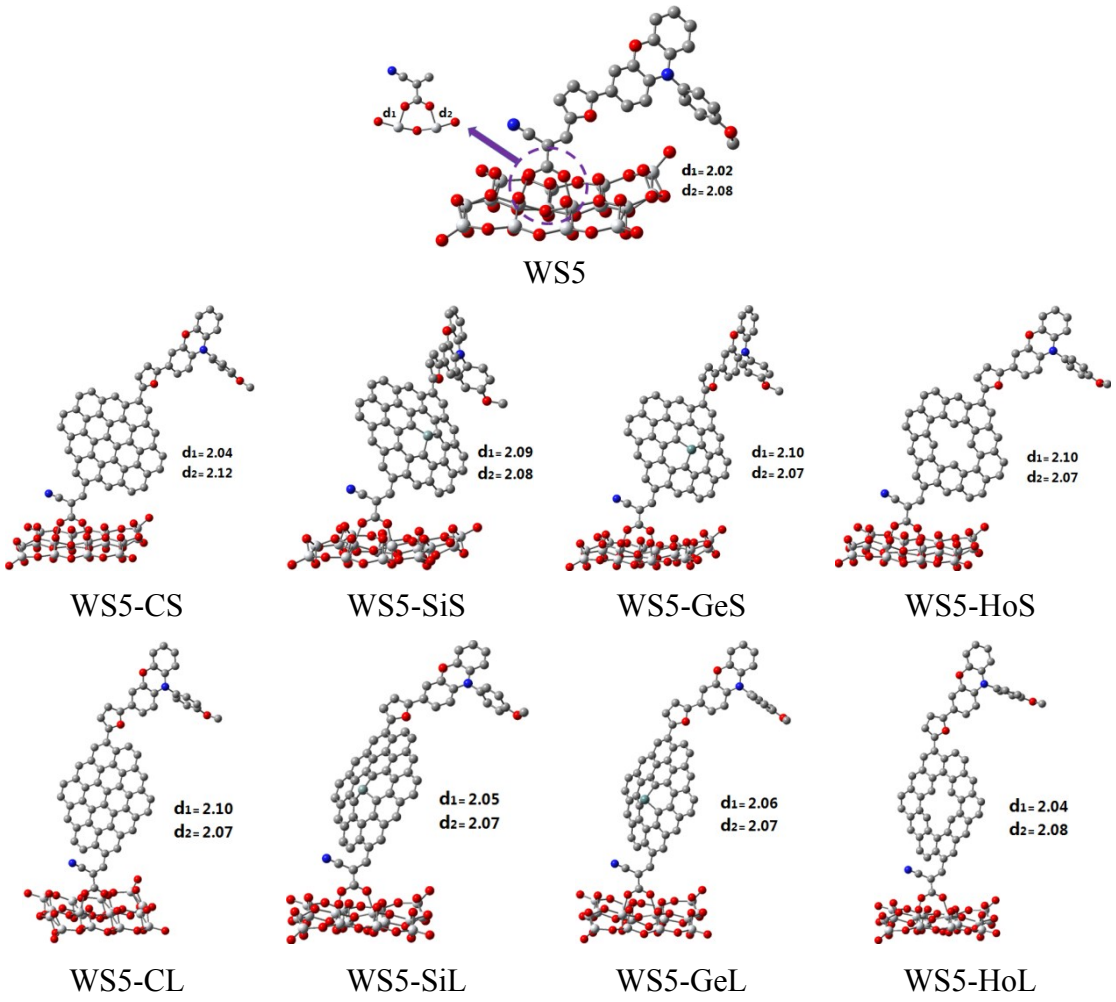

Figure S2 The optimized structures of dyes after binding on the TiO_2

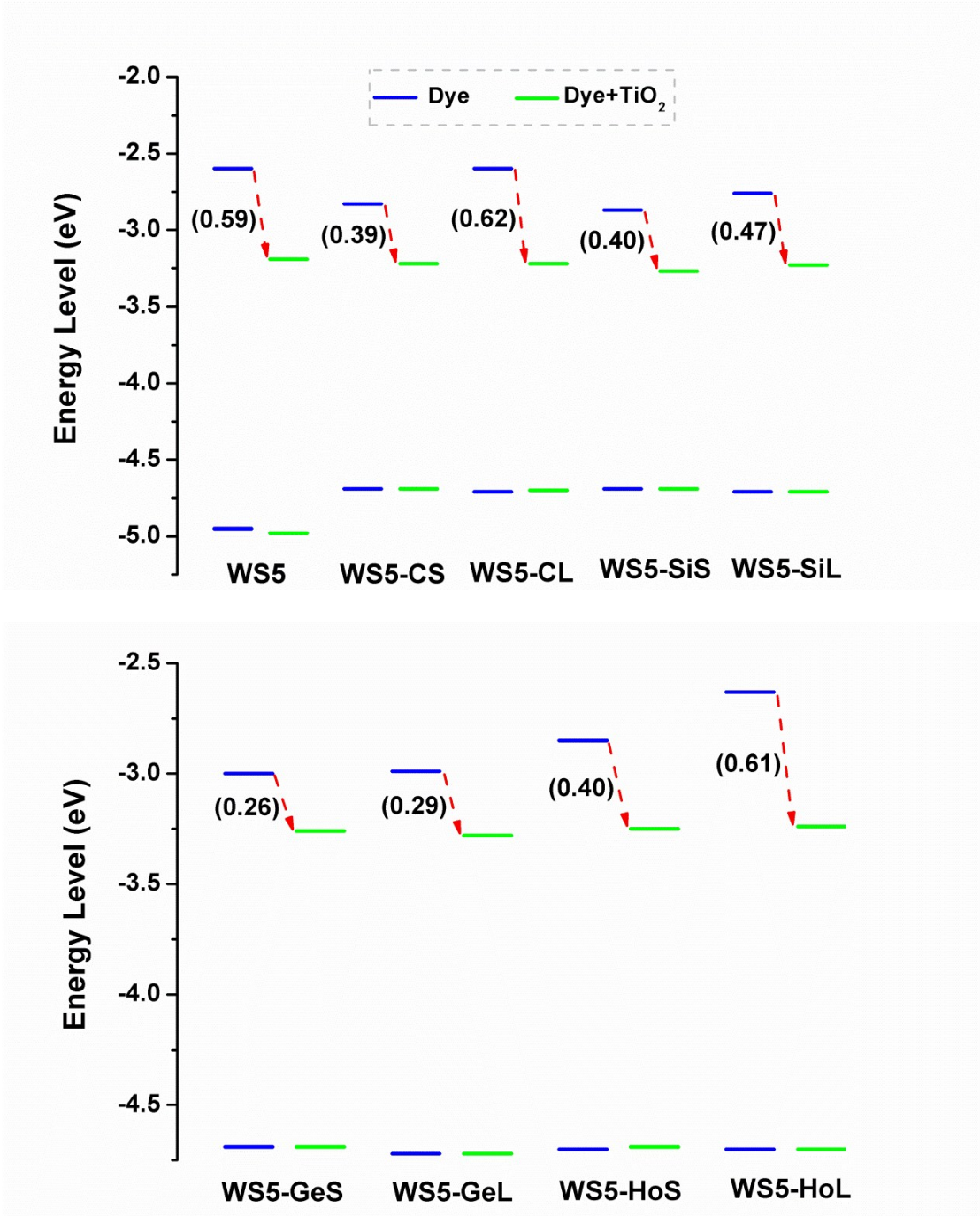

Figure S3 Schematic energy diagram for all studied dyes before and after binding on the TiO_2.

Table S1 The total energies of dyes (a.u.) before and after adsorbed on the $(TiO_2)_{16}$ cluster.

WS5	-1525.3162313	WS5/TiO_2	-5018.3846279
WS5-CS	-3134.4681005	WS5-CS/TiO_2	-6627.5057429
WS5-CL	-3134.4697392	WS5-CL/TiO_2	-6627.5001676
WS5-SiS	-3385.7407301	WS5-SiS/TiO_2	-6878.7713218
WS5-SiL	-3385.7363477	WS5-SiL/TiO_2	-6878.7688738
WS5-GeS	-5171.2387534	WS5-GeS/TiO_2	-8664.0089125
WS5-GeL	-5171.2346168	WS5-GeL/TiO_2	-8664.0037369
WS5-HoS	-3060.5067452	WS5-HoS/TiO_2	-6553.5404044
WS5-HoL	-3060.4980836	WS5-HoL/TiO_2	-6553.5329162

Table S2 The excited state properties of all dyes after binding on the TiO_2.

Dye	E_g (eV)	λ_{max} (nm)	f	Main configuration
WS5	2.38	521	1.0534	H→L/0.67988
WS5-CS	2.80	429	0.8433	H-1→L+1/0.43269
WS5-CL	3.09	401	1.3656	H-2→L/0.55409
WS5-SiS	3.01	412	1.1590	H-2→L/0.35903
WS5-SiL	3.12	397	0.8730	H→L+7/0.42754
WS5-GeS	2.90	428	0.6876	H-4→L/0.41100
WS5-GeL	3.10	399	1.4689	H→L+6/0.37615
WS5-HoS	2.83	438	1.0957	H→L+4/0.38919
WS5-HoL	3.24	383	1.6175	H-1→L+3/0.56504