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D-π-A-π-A 结构有机光敏染料的合成及其在太阳能光电转化和光解水制氢中的应用

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Synthesis of a Novel D-π-A-π-A Organic Sensitizer and Its Application in a Dye-Sensitized Solar Cell and Dye-Sensitized Photocatalytic H2 Production

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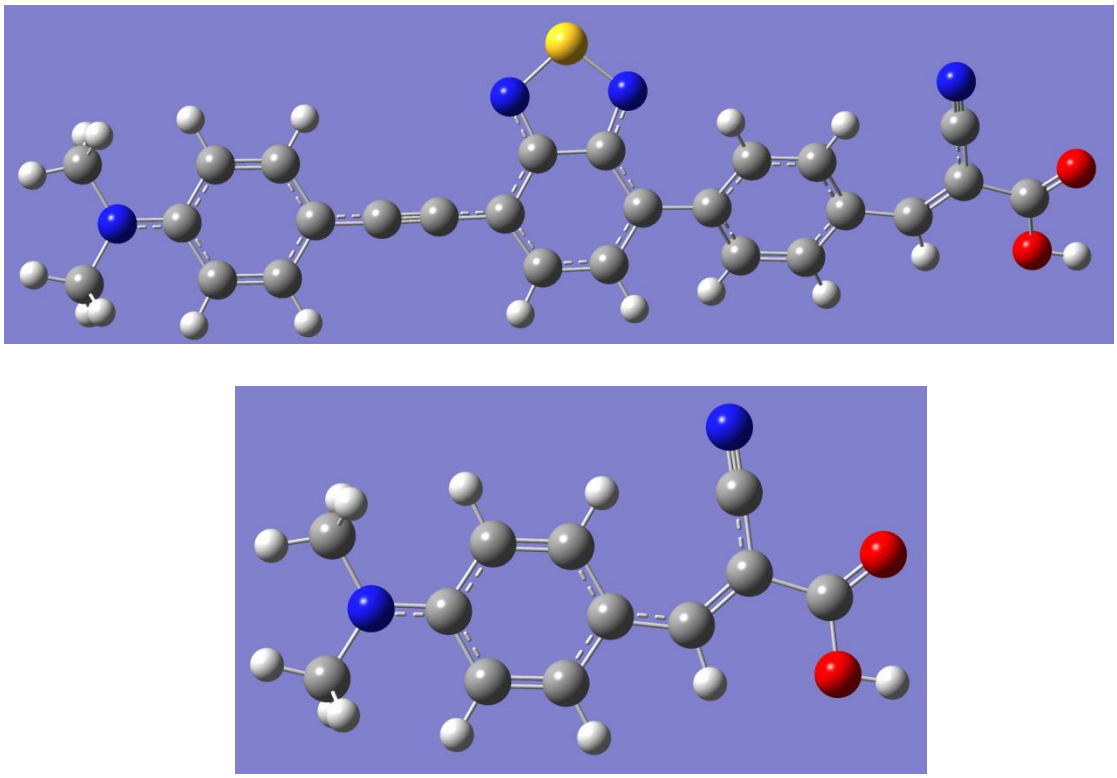
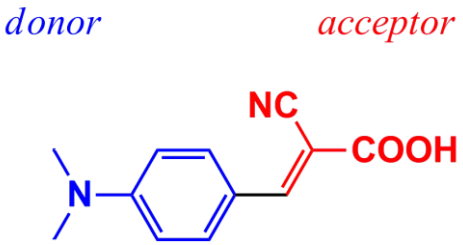


图 S1　OD1 和 OD2 染料的 DFT 优化的分子构型

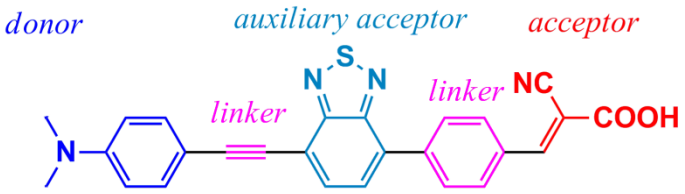
Fig.S1　Optimized molecular configurations of OD1 (top) to OD2 (down) simulated by DFT

表 S1　Mulliken 布居分析 OD1 和 OD2 染料基态(S_0)和激发态(S_1)的电荷分布

Table S1　Ground state (S_0) and excited state (S_1) partial charges of the dye OD1-OD2 from Mulliken Population analysis.



OD1	Partial charges	
	Donor unit	Acceptor unit
Ground State S_0	0.545	-0.545
Excited State S_1	0.636	-0.636



OD2	Partial charges				
	Donor unit	Linker (acetylene)	Auxiliary withdrawing	Linker (phenyl)	Acceptor unit
Ground State S_0	0.128	0.001	-0.120	0.209	-0.224
Excited State S_1	0.423	0.054	-0.289	0.156	-0.344