materials

MDPI

Supplementary Materials

Novel Aggregation-Induced Emission Materials/Cadmium Sulfide Composite Photocatalyst for Efficient Hydrogen Evolution in Absence of Sacrificial Reagent

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DFT Calculation of Band Structure of TEP-Ca

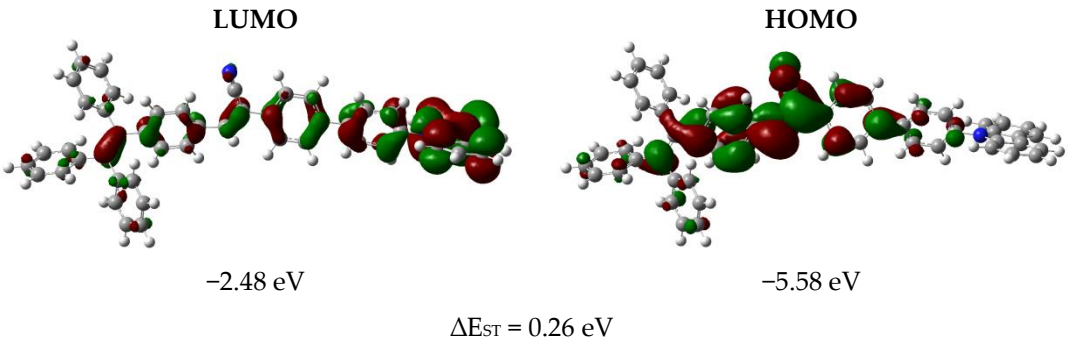

Figure S1. Frontier molecular orbital distributions and energy level diagram of TPE-Ca obtained by DFT calculations (B3LYP/6–31G*).

X-Ray Single-Crystal Diffraction of TEP-Ca

Table S1. The main parameters of TEP-Ca.

Parameter	TPE-Ca
Empirical formula	$C_{53}H_{36}N_2$
Formula weight[g mol^{-1}]	700.84
Crystal system	monoclinic
Space group	P 1 21/n 1
A [Å]	19.8975(12)
B [Å]	9.0425(6)
C [Å]	21.1651(13)
α [°]	-
β[°]	92.499(2)
γ[°]	--
Volume [$Å^3$]	3804.5(4)
Z	4
Density, calcd [g m^{-3}]	1.224
Temperature [K]	220
Unique reflns	6845
Obsdreflns	7994
Parameters	496
R_{int}	0.0636
R[I > 26(I)][a]	0.1698
wR[I > 2(I)]l[b]	0.1830
GOF on F^2	1.024

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