A Strategy for Enhancing the Photoactivity of g-C$_3$N$_4$-based Single-atom Catalysts via Sulphur Doping: A Theoretical Study

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Table S1 Structure parameters, bond lengths (Å) and bond populations of g-C_3N_4, S-g-C_3N_4, Pt/g-C_3N_4 and Pt/S-g-C_3N_4.

Species	Structure parameters			Bond	Bond length/Å	Bond populations
	a/Å	b/Å	c/Å			
g-C_3N_4	7.15	7.15	7.50	C1-N1	1.39	0.81
				C1-N2	1.33	1.03
				C2-N2	1.34	1.04
				C2-N3	1.47	0.76
S-g-C_3N_4	7.16	7.14	7.52	C1-N1	1.35	0.83
				C1-S	1.74	0.44
				C2-S	1.79	0.65
				C2-N3	1.44	0.79
Pt/ g-C_3N_4	7.17	7.16	7.54	C1-N1	1.36	0.84
				C1-N2	1.33	1.07
				C2-N2	1.35	0.97
				C2-N3	1.45	0.80
				N4-Pt	2.18	0.20
				N6-Pt	2.19	0.20
Pt/ S-g-C_3N_4	6.95	6.70	9.33	C1-N1	1.36	0.90
				C1-S	1.81	0.59
				C2-S	1.86	0.51
				C2-N3	1.44	0.75
				S-Pt	2.16	0.44
				N5-Pt	2.19	0.23

Table S2 Mulliken charge populations of $g\text{-}C_3N_4$, $S\text{-}g\text{-}C_3N_4$, $Pt/g\text{-}C_3N_4$ and $Pt/S\text{-}g\text{-}C_3N_4$.

Species	Atom	Mulliken charge population			
		s	p	d	Charge/|e|
$g\text{-}C_3N_4$	C1	0.91	2.58	0	0.51
	C2	0.94	2.58	0	0.48
	N1	1.41	3.92	0	-0.33
	N2	1.53	3.85	0	-0.39
	N3	1.43	3.87	0	-0.30
	N4	1.53	3.85	0	-0.39
	N5	1.53	3.85	0	-0.39
	N6	1.53	3.85	0	-0.39
$S\text{-}g\text{-}C_3N_4$	C1	1.05	2.77	0	0.18
	C2	1.05	2.80	0	0.15
	N1	1.41	3.93	0	-0.34
	N3	1.43	3.86	0	-0.28
	N4	1.50	3.96	0	-0.46
	N5	1.54	3.86	0	-0.40
	N6	1.52	3.87	0	-0.40
	S	1.82	3.72	0	0.46
$Pt/g\text{-}C_3N_4$	C1	0.91	2.62	0	0.47
	C2	0.94	2.61	0	0.45
	N1	1.40	3.95	0	-0.35
	N2	1.52	3.92	0	-0.44
	N3	1.42	3.87	0	-0.29
	N4	1.53	3.90	0	-0.44
	N5	1.51	3.92	0	-0.43
	N6	1.53	3.90	0	-0.44
	Pt	0.57	-0.16	8.81	0.77
$Pt/S\text{-}g\text{-}C_3N_4$	C1	1.06	2.75	0	0.19
	C2	1.07	2.79	0	0.14
	N1	1.41	3.92	0	-0.32
	N3	1.40	3.89	0	-0.28
	N4	1.55	3.86	0	-0.42
	N5	1.54	3.92	0	-0.46
	N6	1.53	3.87	0	-0.40
	S	1.78	3.86	0	0.37
	Pt	0.72	-0.12	9.18	0.22
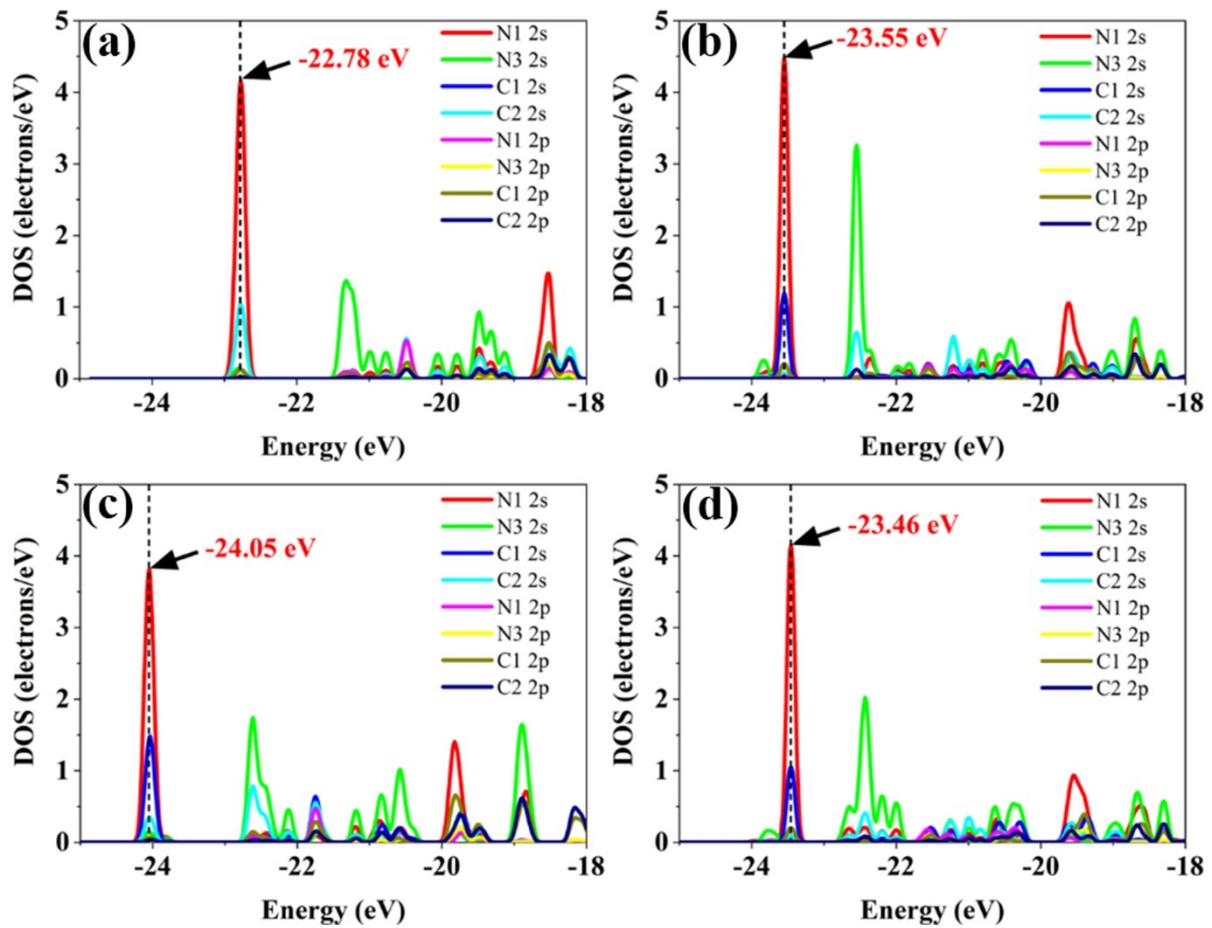
Fig. S1 Density of states of deep states of g-C_3N_4 (a), S-g-C_3N_4 (b), Pt/g-C_3N_4 (c) and Pt/S-g-C_3N_4 (d), where the N1 2s state marked by an arrow is used as the reference.
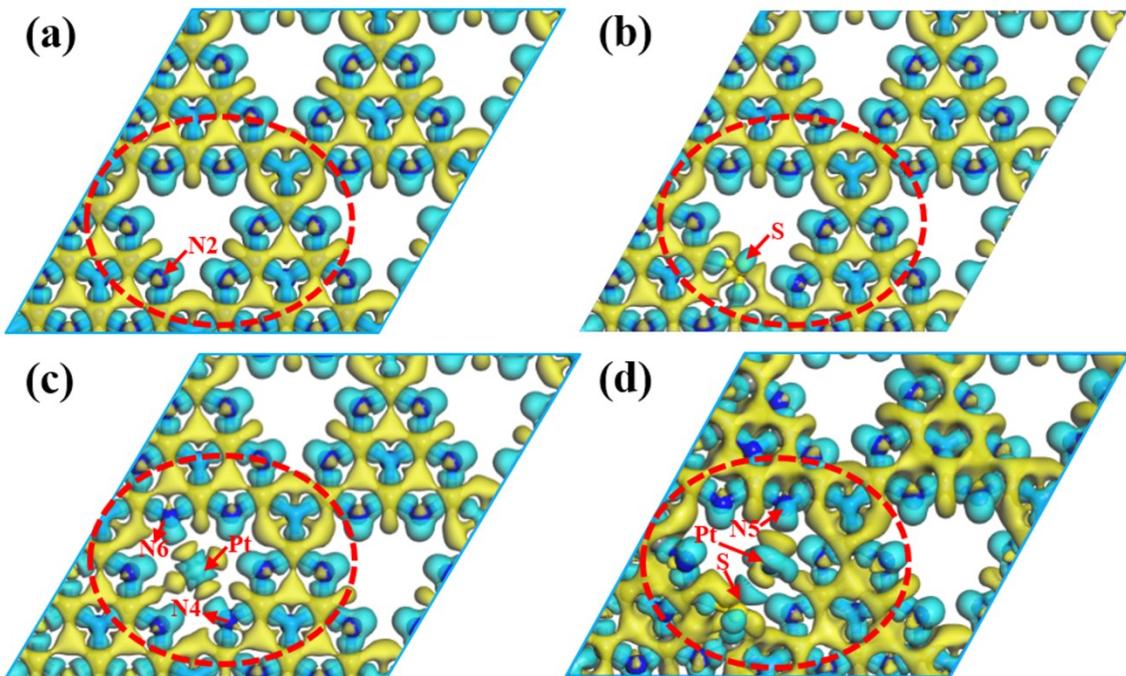
Fig. S2 Calculated electron density difference of g-C$_3$N$_4$ (a), S-g-C$_3$N$_4$ (b), Pt/g-C$_3$N$_4$ (c)and Pt/S-g-C$_3$N$_4$ (d). The cyan region indicates electron accumulation, and the olive color region represents electron depletion. The isovalue is set as 0.05 electron/Å^3.
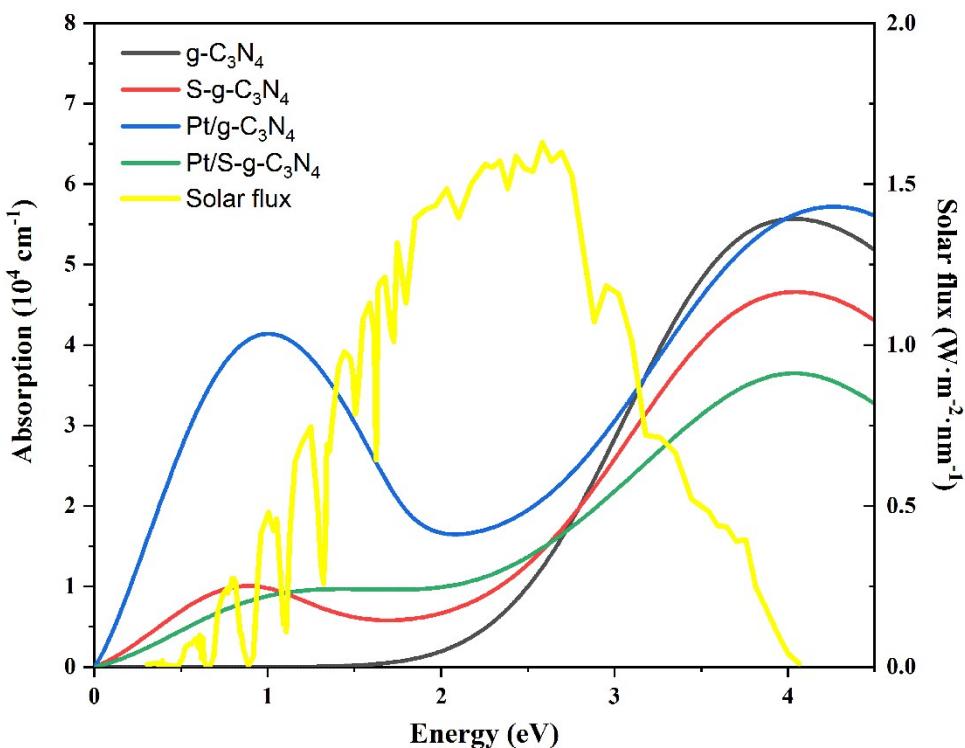

Fig. S3 Absorption spectrum of g-C$_3$N$_4$, S-g-C$_3$N$_4$, Pt/g-C$_3$N$_4$ and Pt/S-g-C$_3$N$_4$.