Supporting Information for

Tunable optical and photocatalytic performance promoted by nonstoichiometric control and site-selective codoping of travillent ions in $NaTaO_3$

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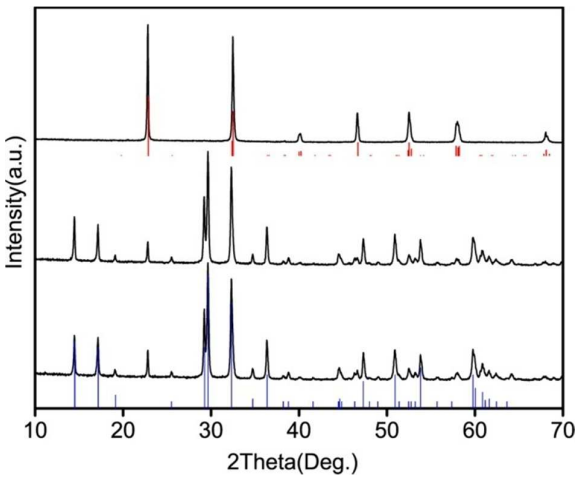

Figure S1 XRD patterns of Eu^{3+} doped $NaTaO_3$ with different Na/Ta initial molar ratio of 2.5(a), 1.5 (b) and 1 (c). Vertical bars represent the standard diffraction data from JCPDS file for $NaTaO_3$ (up one, 25-0863) and $Na_2Ta_4O_{11}$ (down one, 84-0810).

Table S2 Lattice parameters of pure $NaTaO_3$ and doped $NaTaO_3$ based density functional theory (DFT) calculations and experimental data

Calculated data	Formula	Lattice volume (Å^3)	a (Å)	b (Å)	c (Å)
	$NaTaO_3$	259.11	5.8636	7.9890	5.5313
	Na_i	272.15	5.7789	8.1460	5.7813
	Nai-Eu@Ta	272.49	5.8150	8.1442	5.7538
	Eu@Ta	282.75	5.7307	8.2399	5.9879
	Eu@Na	270.90	5.6796	8.1590	5.8462
Selected experimental data	Na/Ta molar ratio	Lattice volume (Å^3)	a (Å)	b (Å)	c (Å)
	1.041	235.30	5.5136	7.7825	5.4842
	1.046	235.72	5.4898	7.7797	5.5190

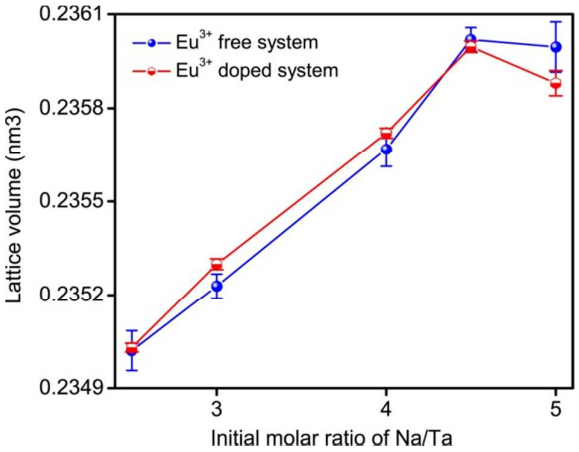

Figure S3 Lattice volume of Eu^{3+} doped and Eu^{3+} free $NaTaO_3$ as a function of Na/Ta initial molar ratio.

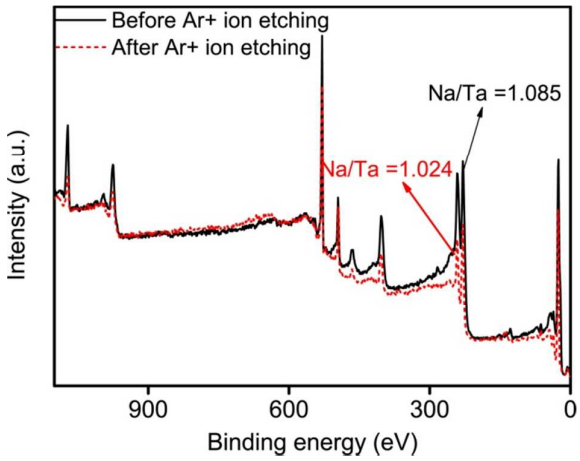

Figure S4 XPS spectra of Eu^{3+} doped NaTaO3 with Na/Ta molar ratio of 1.041 before and after Ar^{+} ions etching.

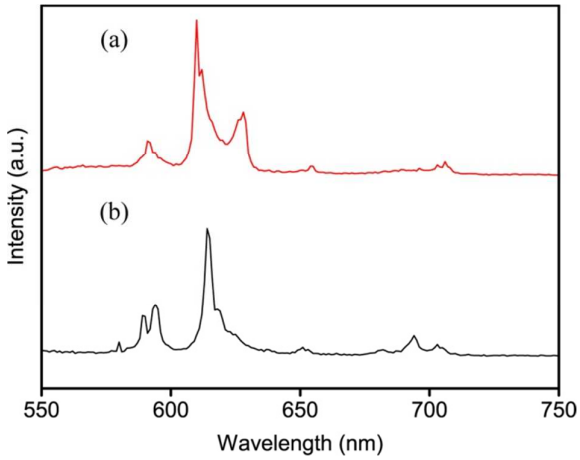

Figure S5 Emission spectra of surface Eu^{3+} doped $NaTaO_3$ (a) and Eu^{3+} doped $NaTaO_3$ with Na/Ta initial molar ratio of 2.5.

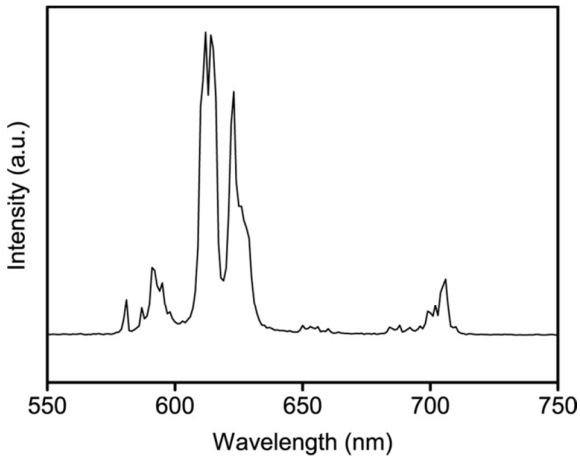

Figure S6 Emission spectrum of Eu_2O_3 under 395 nm excitation.

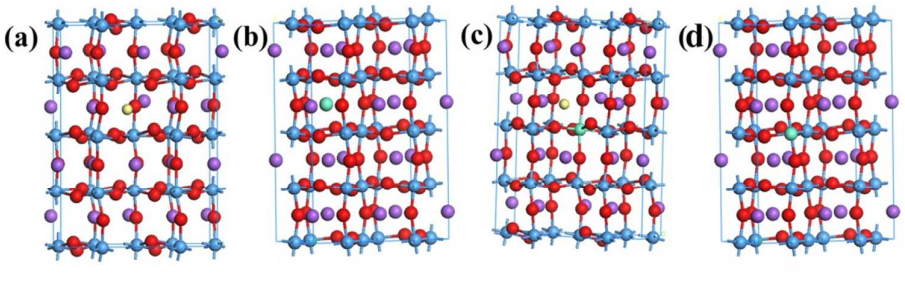

Figure S7 The supercell model proposed for doped $NaTaO_3$: Na at an interstitial site (a), Eu at Na site (b), the dual substitute model by substituting Na at interstitial site and Eu at Ta site (c) and Eu at Ta site (d).

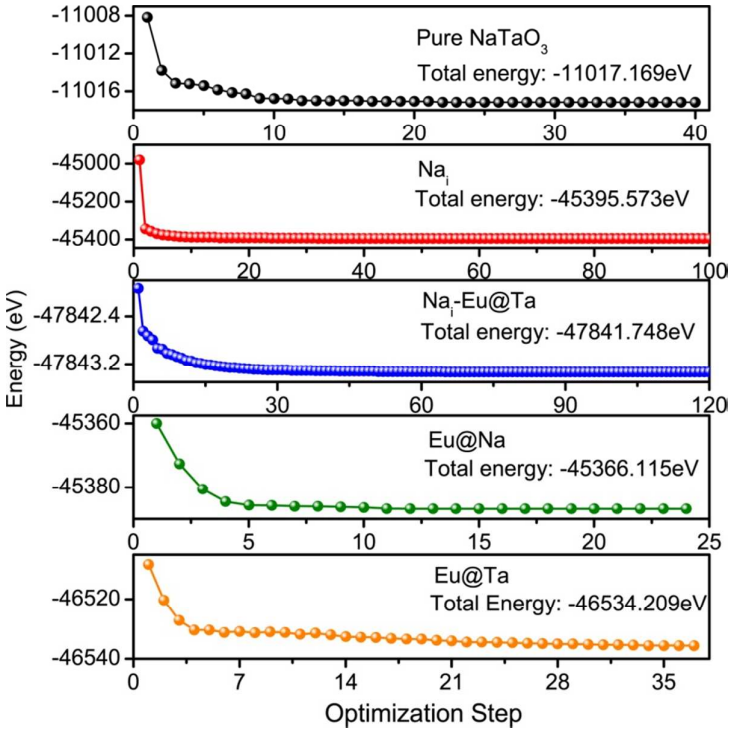

Figure S8 Total energy and energetic convergence data of all calculated models.

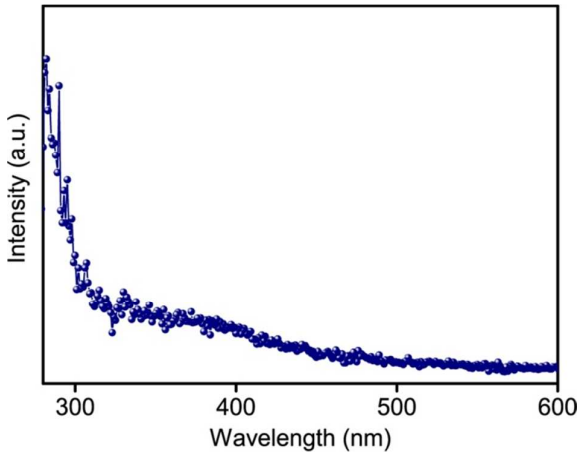

Figure S9 UV-vis reflectance spectra of undoped $NaTaO_3$.

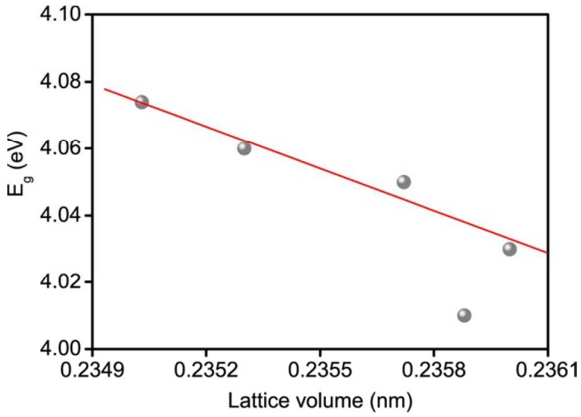

Figure S10 Correlation between the band gap energies, E_g, and the lattice volume of Eu^{3+} doped $NaTaO_3$.

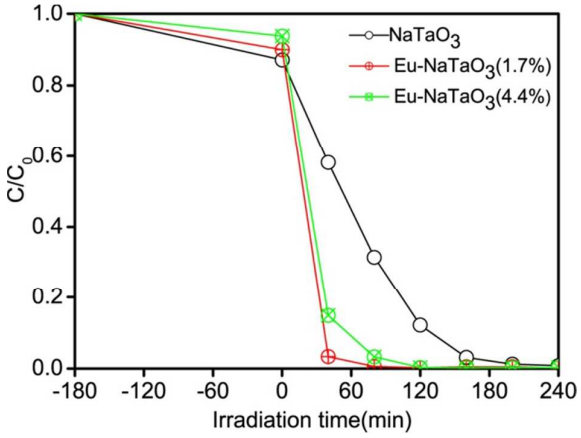

Figure S11 Normalized concentration of MB versus UV light irradiation time of Eu^{3+} doped $NaTaO_3$ prepared with initial Na/Ta molar ratio of 2.5.

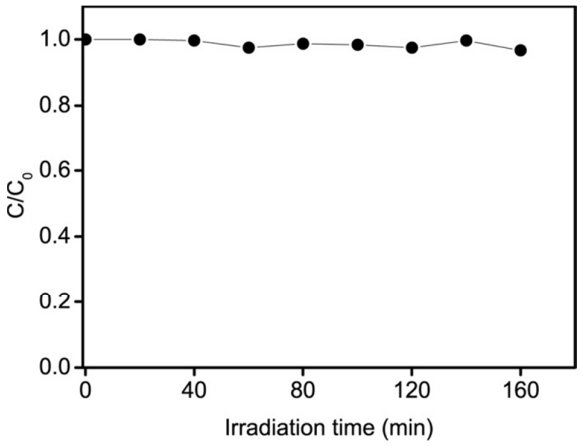

Figure S12 Normalized concentration of MB versus UV light irradiation time in the absence of Eu^{3+} doped $NaTaO_3$.

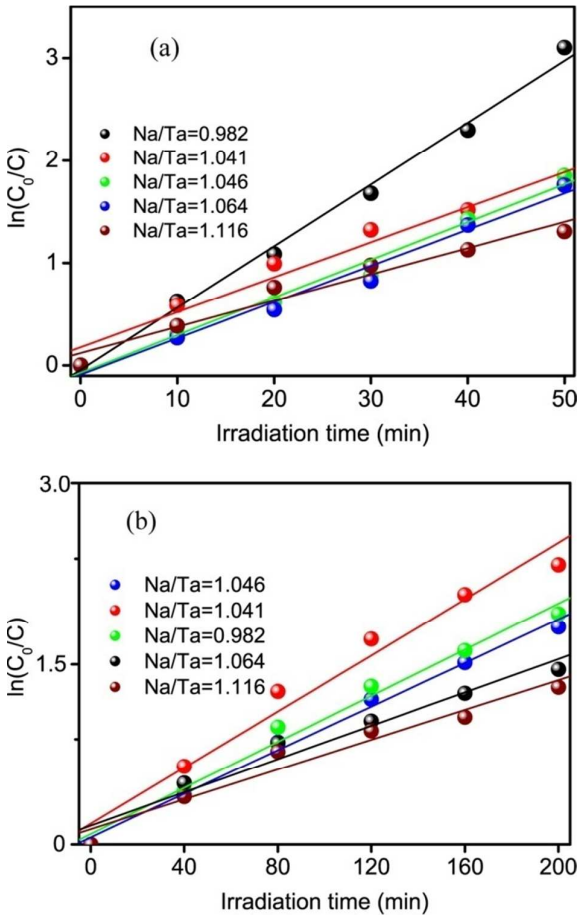

Figure S13 The $\ln(C_0/C)$ versus time curves of MB photodegradation over Eu^{3+} doped $NaTaO_3$ under UV light irradiation (a) and visible light irradiation (b).