Electronic Supplementary Information (ESI)

Density functional theory (DFT) investigation on the structure and photocatalysis properties of double-perovskite $Gd_{1-x}Ca_xBaCo_2O_{5+\delta}$ ($0 \le x \le 0.4$)

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Table S1. Lattice parameters of $Gd_{1-x}Ca_xBaCo_2O_{5+\delta}$ ($0 \le x \le 0.5$)

x	Lattice parameters			Cell volume (Å)^3
	a (Å)	b (Å)	c (Å)	
0	3.91	3.87	7.54	114.12
0.1	3.92	3.87	7.55	114.43
0.2	3.91	3.88	7.54	114.48
0.3	3.92	3.86	7.55	114.50
0.4	3.92	3.88	7.55	114.72

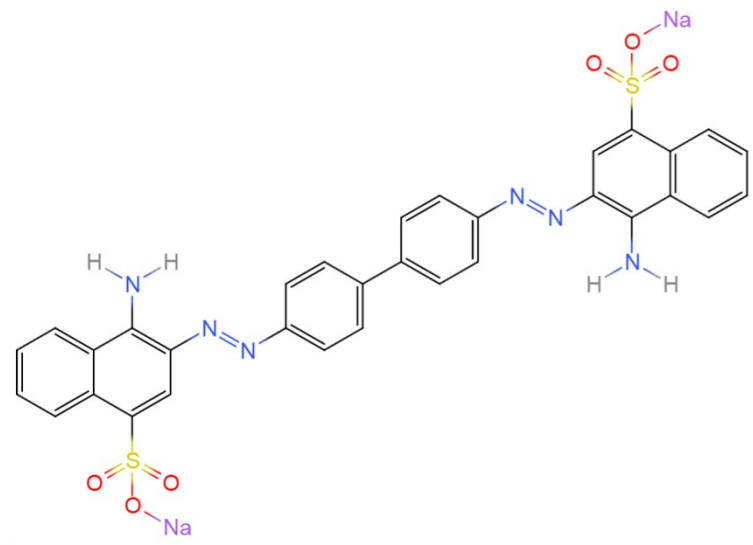

Fig. S1. Chemical structural molecular formula of congo red.

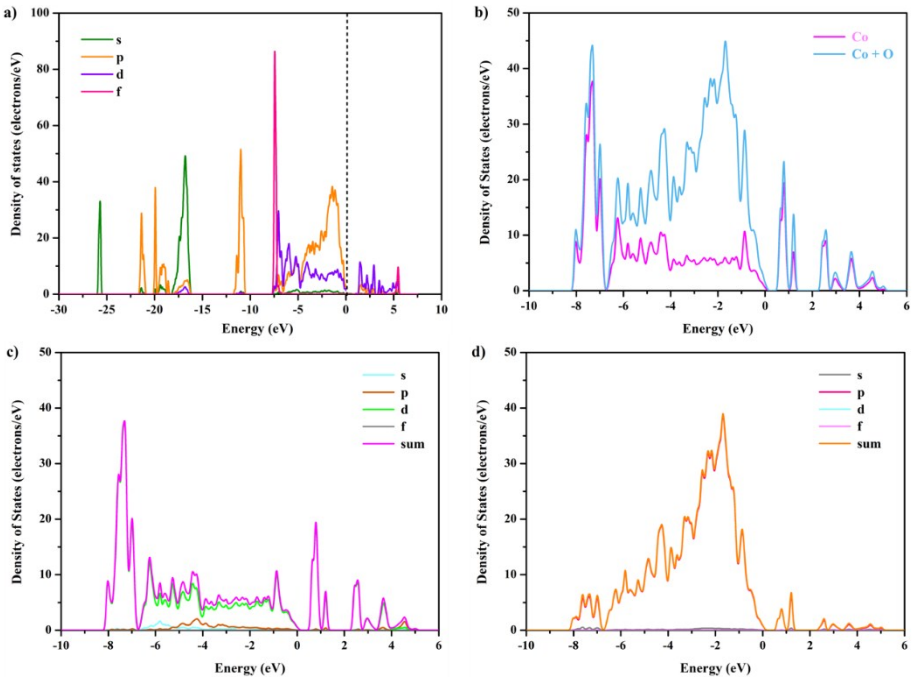

Fig. S2. Electronic density of states of the simulated $GdBaCo_2O_{5+\delta}$: (a) the total density of states, (b) Sum of Co and O density of states, (c) the partial DOS (PDOS) for Co, (d) the partial DOS (PDOS) for O. $\left(U_{3d}^{Co}, J_{3d}^{Co}\right) = (5,0)$ eV in all cases. The Fermi energy is set at 0 eV.

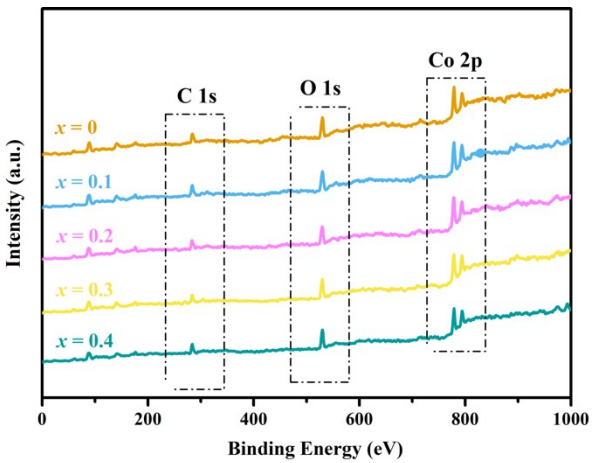

Fig. S3. XPS spectra for the $Gd_{1-x}Ca_xBaCo_2O_{5+\delta}$（$0 \le x \le 0.4$）specimens: wide-survey spectrum (the binding energy is from 0 to 1000 eV)

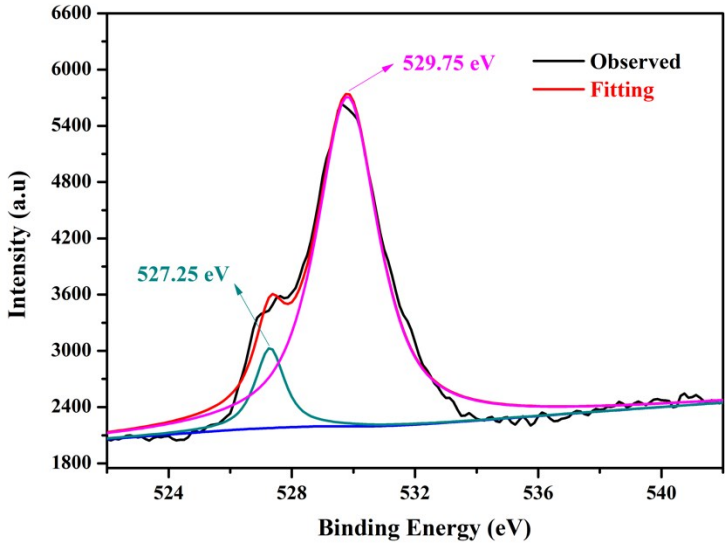

Fig. S4. XPS spectra for $Gd_{0.8}Ca_{0.2}BaCo_2O_{5+\delta}$: O-1*s* core-level (the binding energy is from 522 to 542 eV).

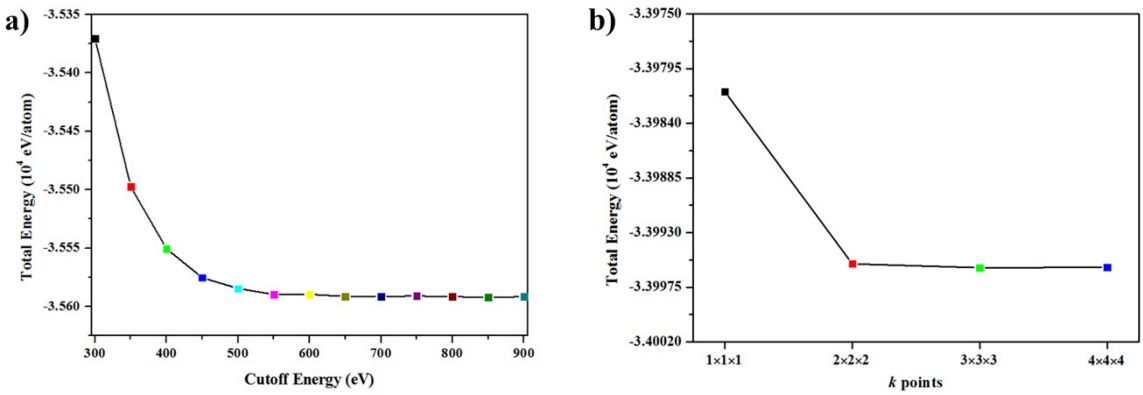

Fig. S5. Statistical curve of convergence test results: a) cutoff energy; b) *k* points.