Supporting Information for

The impact of metal cations on photochemical properties of hybrid heterostructures with infinite alkaline-earth metal oxide clusters

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1. Single-crystal X-ray diffraction analysis

Table S1 Crystal data and structure refinements for hybrids 1 and 2.

Complex	**1**	**2**
Empirical formula	$C_{24}CaH_{26}N_4O_9$	$C_{24}H_{26}N_4O_9Sr$
Formula weight	554.57	602.11
Temperature/K	293(2)	293(2)
Crystal system	tetragonal	tetragonal
Space group	$I4_1/a$	$I4_1/a$
a/Å	28.1585(17)	28.614(4)
b/Å	28.1585(17)	28.614(4)
c/Å	13.4560(16)	13.749(3)
α/°	90	90
β/°	90	90
γ/°	90	90
Volume/$Å^3$	10669.3(18)	11258(4)
Z	16	16
$\rho_{calc}g/cm^3$	1.381	1.421
μ/mm^{-1}	0.293	1.970
F(000)	4640	4928.0
Radiation	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.655 to 25.027	3.130 to 25.023
Reflections collected	23227	42452
Independent reflections	4698 [R_{int} = 0.1125]	4971 [R_{int} = 0.0945]
Data/restraints/parameters	4698/0/303	4971/339/302
Goodness-of-fit on F^2	0.992	1.029
Final R indexes [I>=2σ (I)]	R_1 = 0.0702, wR_2 = 0.1540	R_1 = 0.0563, wR_2 = 0.1491
Final R indexes [all data]	R_1 = 0.1356, wR_2 = 0.1773	R_1 = 0.0869, wR_2 = 0.1652
Largest diff. peak/hole / e $Å^{-3}$	0.243/-0.195	0.776/-0.550

2. Infrared spectral analysis

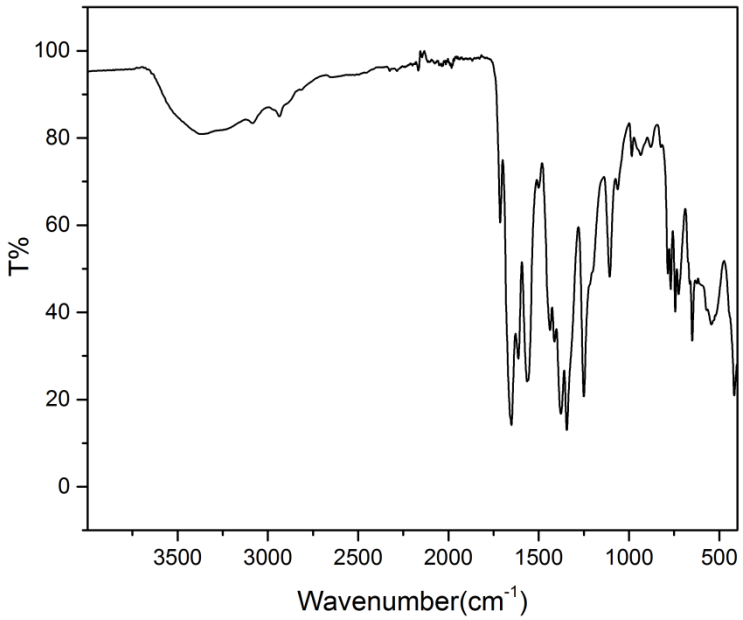

Figure S1. Infrared spectrum of hybrid **1**

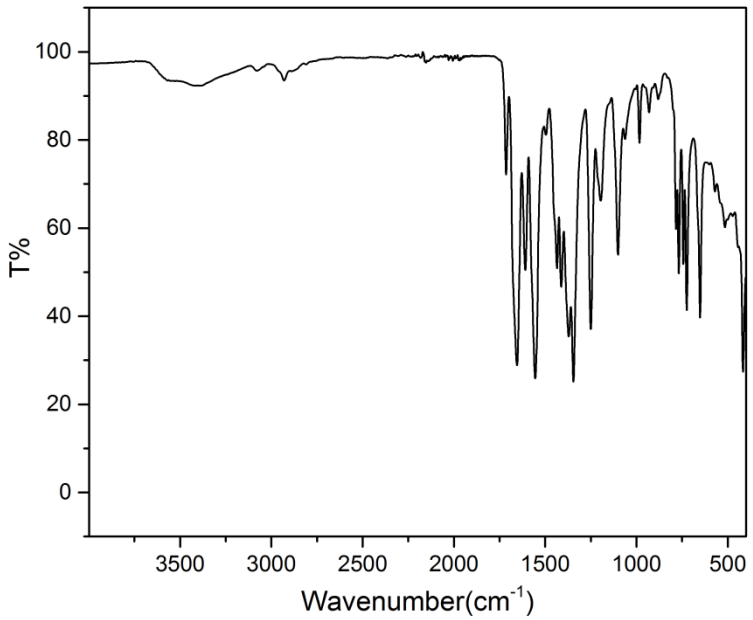

Figure S2. Infrared spectrum of hybrid **2**

3. Electron paramagnetic resonance (EPR) spectra

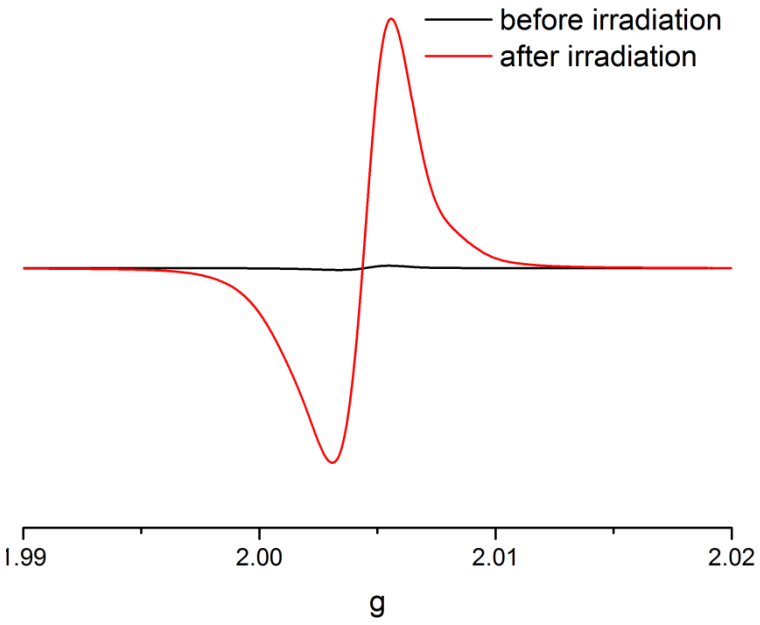

Figure S3. EPR spectra of hybrid **1** before and after irradiation by Xenon Lamp

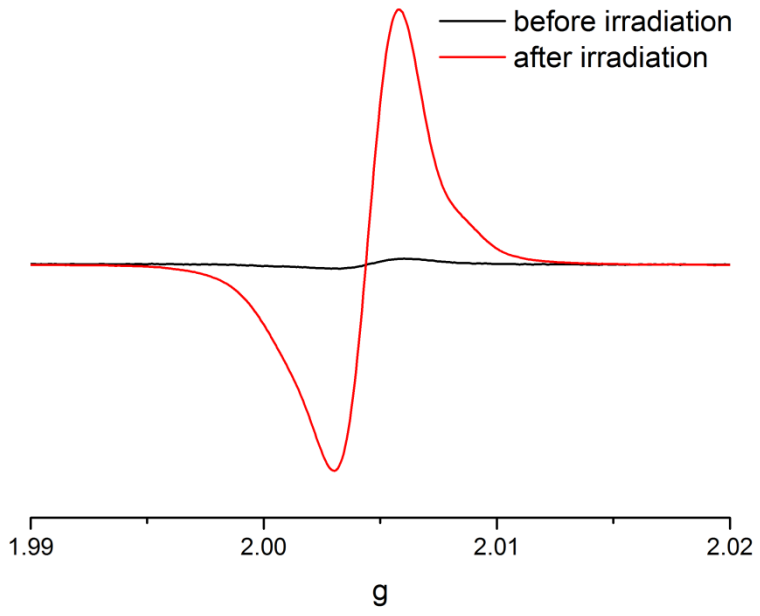

Figure S4. EPR spectra of hybrid **2** before and after irradiation by Xenon Lamp

4. Powder X-ray diffraction analysis

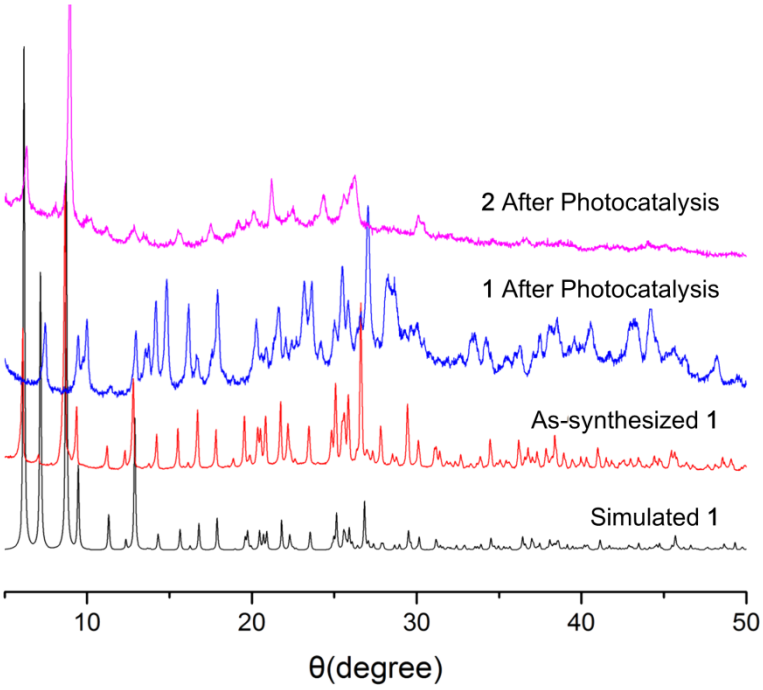

Figure S5. PXRD patterns of hybrids **1** and **2** before and after the photocatalytic degradation of MB.