Supporting Information

Accelerated Perovskite Discovery: Screening New Catalysts for Photocatalytic Methylene Blue Degradation

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Table S1: List of chemicals utilized in the present study.

Chemical	Formula	Supplier	M (g/mol)	Purity (%)
Magnesium nitrate hexahydrate	$Mg(NO_3)_2{\cdot}6H_2O$	Wako	256.41	
Aluminium nitrate nonahydrate	$Al(NO_3)_3{\cdot}9H_2O$	Kanto Chemical	375.13	>98
Tetraethyl orthosilicate (III)	$Si(OC_2H_5)_4$	Tokyo Chemical Industry	208.33	>98
Calcium nitrate tetrahydrate	$Ca(NO_3)_2{\cdot}4H_2O$	Kanto Chemical	236.15	>98.5
Titanium(IV) isopropoxide	$C_{12}H_{28}O_4Ti$	Sigma-Aldrich	284.22	>97
Iron(III) nitrate nonahydrate	$Fe(NO_3)_3{\cdot}9H_2O$	Sigma-Aldrich	404.00	≥99.95
Cobalt(II) nitrate hexahydrate	$Co(NO_3)_2{\cdot}6H_2O$	Sigma-Aldrich	291.03	≥98
Nickel(II) nitrate hexahydrate	$Ni(NO_3)_2{\cdot}6H_2O$	Wako	290.79	99.9
Copper(II) nitrate trihydrate	$Cu(NO_3)_2{\cdot}3H_2O$	Sigma-Aldrich	241.60	>99
Zinc nitrate hexahydrate	$Zn(NO_3)_2{\cdot}6H_2O$	Sigma-Aldrich	297.49	98
Gallium nitrate	$Ga(NO_3)_3{\cdot}xH_2O$	Kojundo	255.74	99.999

Strontium nitrate	$Sr(NO_3)_2$	Kanto Chemical	211.63	
Yttrium(III) nitrate hexahydrate	$Y(NO_3)_3 \cdot 6H_2O$	Sigma-Aldrich	383.01	99.8
Zirconium oxynitrate	$ZrO(NO_3)_2 \cdot 2H_2O$	Nacalai tesque	267.26	≥98.0
Niobium pentaethoxide	$Nb(OC_2H_5)_5$	Kojundo	318.21	99.99
Indium(III) nitrate trihydrate	$In(NO_3)_3 \cdot 3H_2O$	Wako	354.88	97
Barium nitrate	$Ba(NO_3)_2$	Sigma-Aldrich	261.34	99.999
Tantalum pentaethoxide	$Ta(OC_2H_5)_5$	Kojundo	406.25	99.999
Ammonium tungstate pentahydrate	$(NH4)_6H_2W_{12}O_{40} \cdot xH_2O$	Sigma-Aldrich	2956.30	>85
Lanthanum(III) nitrate hexahydrate	$La(NO_3)_3 \cdot 6H_2O$	Kanto Chemical	433.01	>99.0
Cerium(III) nitrate hexahydrate	$Ce(NO_3)_3 \cdot 6H_2O$	Sigma-Aldrich	434.22	99
Praseodymium(III) nitrate hexahydrate	$Pr(NO_3)_3 \cdot 6H_2O$	Stream Chemicals	435.02	99.9
Neodymium(III) nitrate hexahydrate	$Nd(NO_3)_3 \cdot 6H_2O$	Sigma-Aldrich	438.35	99.9
Citric acid	$C_6H_8O_7$	Sigma-Aldrich	192.12	>99.5

Table S2: Selected Combinations from 23 elements.

No.	**Combination**
1.	$NdFeO_3$
2.	$BaZrO_3$
3.	$PrFeO_3$
4.	$BaTiO_3$
5.	$CaTiO_3$
6.	$LaInO_3$
7	$PrInO_3$
8.	$LaFeO_3$
9.	$BaNiO_3$
10.	$MgTiO_3$

11.	$CaZrO_3$
12.	$InGaO_3$
13.	$BaCeO_3$
14.	$SrZrO_3$
15.	$LaCoO_3$
16.	$LaAlO_3$
17.	$SrTiO_3$

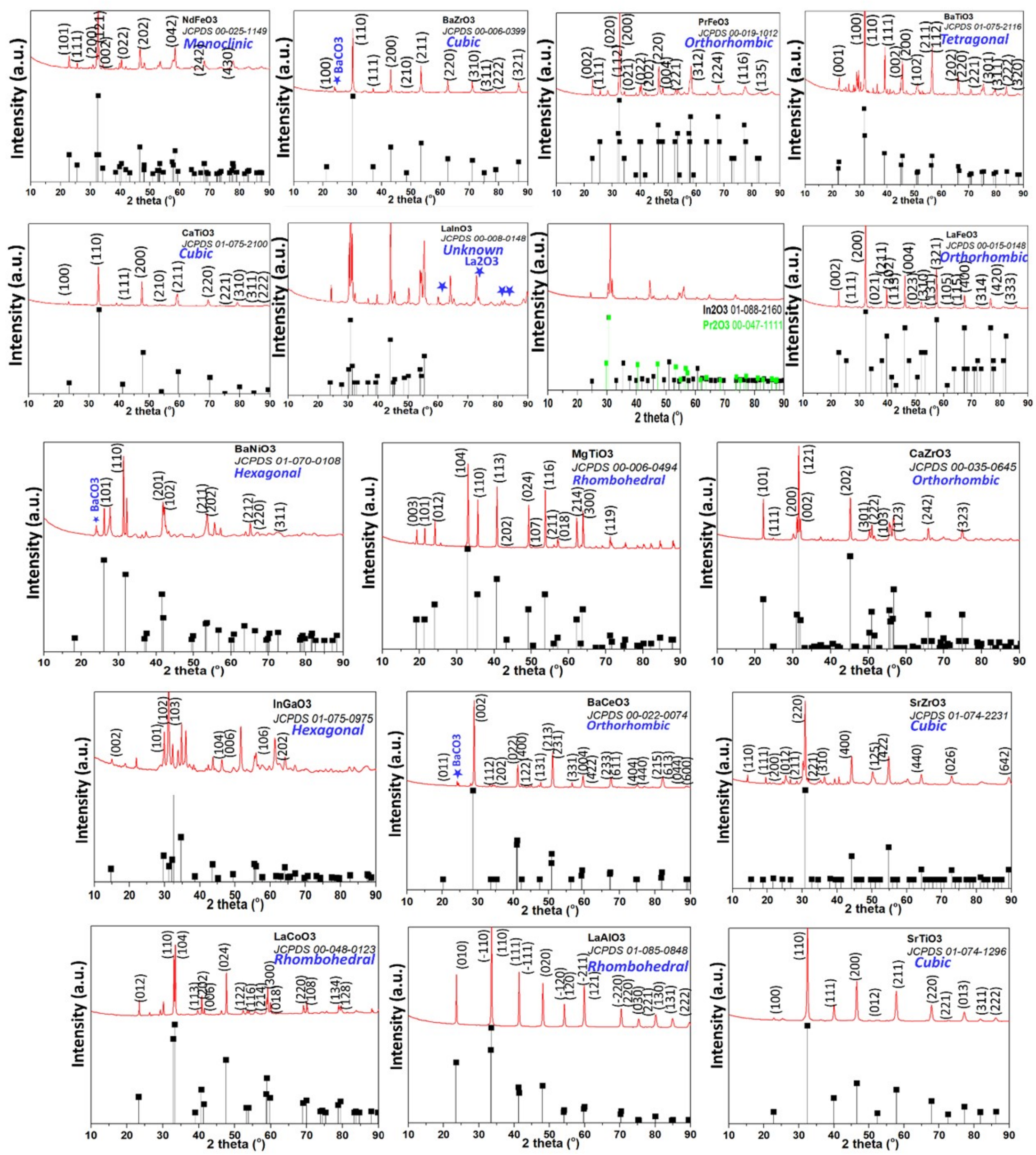

Figure S1: PXRD plots of 17 combinations.

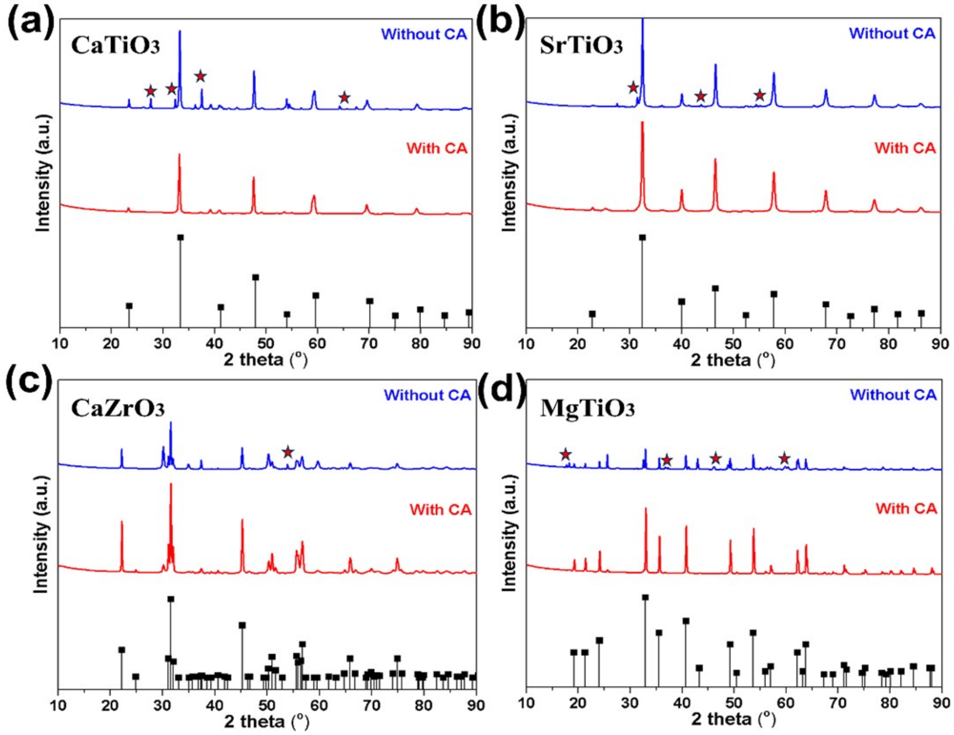

Figure S2: XRD plots of (a) $CaTiO_3$, (b) $SrTiO_3$, (c) $CaZrO_3$, and (d) $MgTiO_3$, synthesized with and without CA. The symbol ★ represents the presence of extra peaks in perovskites synthesized in the absence of CA.

Table S3: Summarized data of BET surface area and total pore volume

Combination	**BET surface area (m^2/g)**		**Total pore volume (cm^3/g)**	
	w/o CA	*with CA*	*w/o CA*	*with CA*
$CaTiO_3$	2.036	10.885	0.0022	0.0124
$SrTiO_3$	1.401	14.106	0.0018	0.0190
$CaZrO_3$	0.862	3.158	0.0009	0.0039
$MgTiO_3$	0.931	1.126	0.0014	0.0015

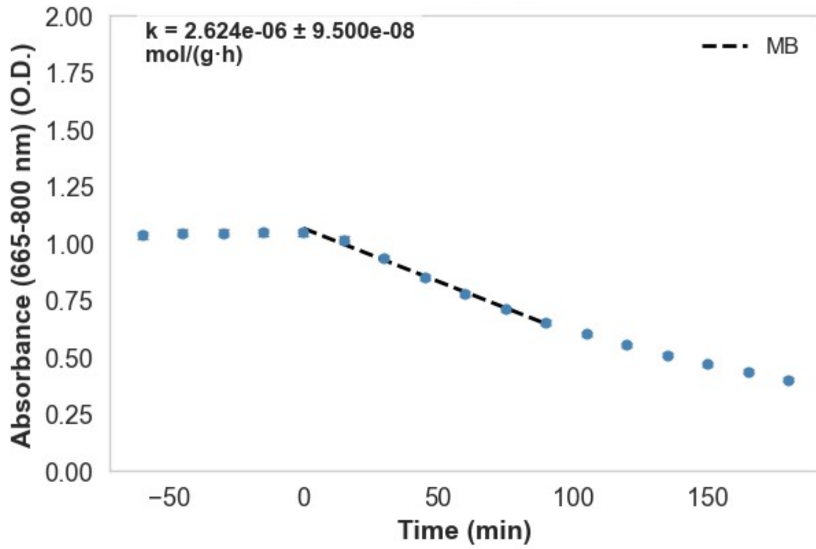

Figure S3: Photocatalytic degradation of MB alone.

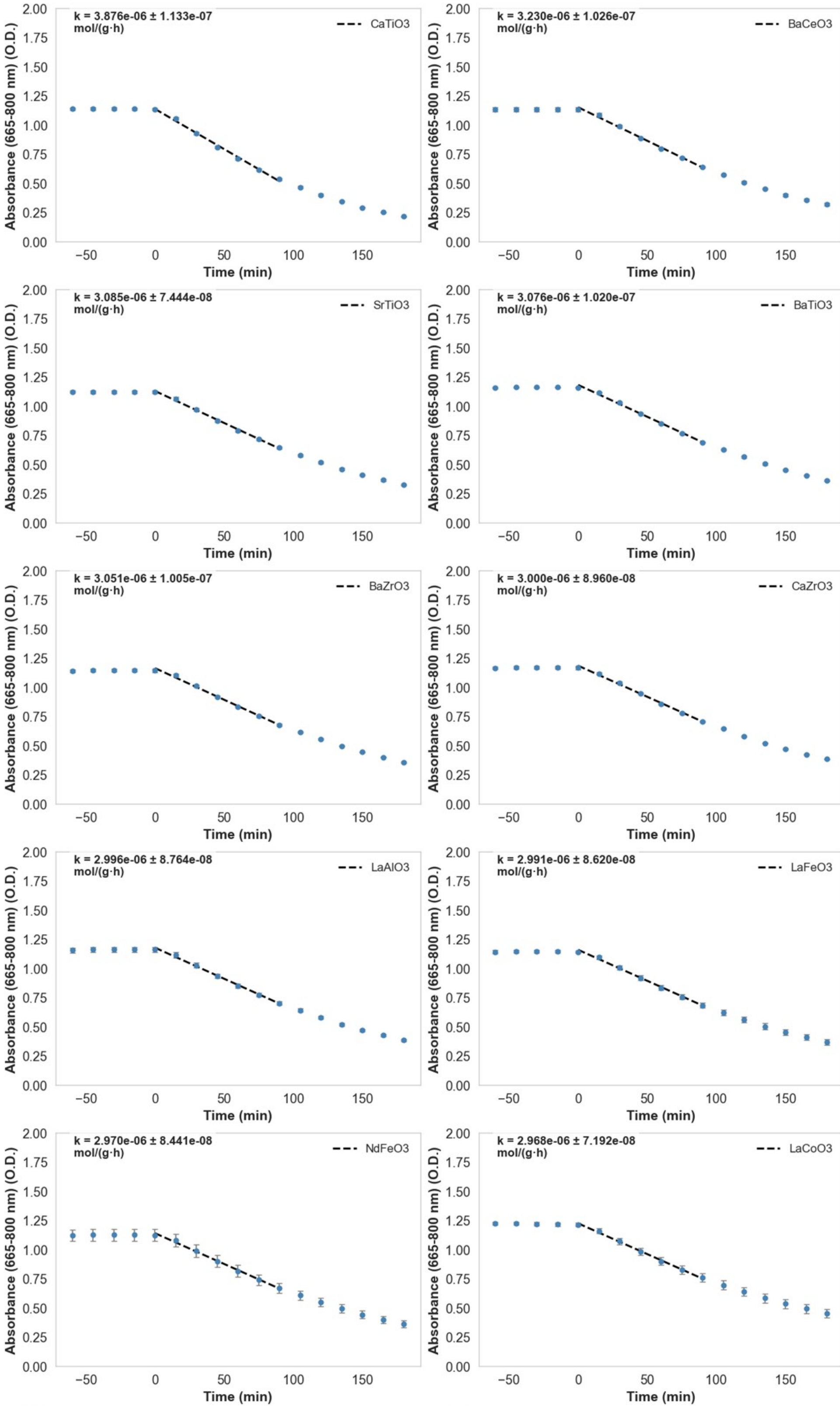
k = 3.876e-06 ± 1.133e-07
mol/(g·h)
CaTiO3
k = 3.230e-06 ± 1.026e-07
mol/(g·h)
BaCeO3
k = 3.085e-06 ± 7.444e-08
mol/(g·h)
SrTiO3
k = 3.076e-06 ± 1.020e-07
mol/(g·h)
BaTiO3
k = 3.051e-06 ± 1.005e-07
mol/(g·h)
BaZrO3
k = 3.000e-06 ± 8.960e-08
mol/(g·h)
CaZrO3
k = 2.996e-06 ± 8.764e-08
mol/(g·h)
LaAlO3
k = 2.991e-06 ± 8.620e-08
mol/(g·h)
LaFeO3
k = 2.970e-06 ± 8.441e-08
mol/(g·h)
NdFeO3
k = 2.968e-06 ± 7.192e-08
mol/(g·h)
LaCoO3
Absorbance (665-800 nm) (O.D.)
Time (min)

Figure S4: Photocatalytic degradation of MB in the presence of catalysts.

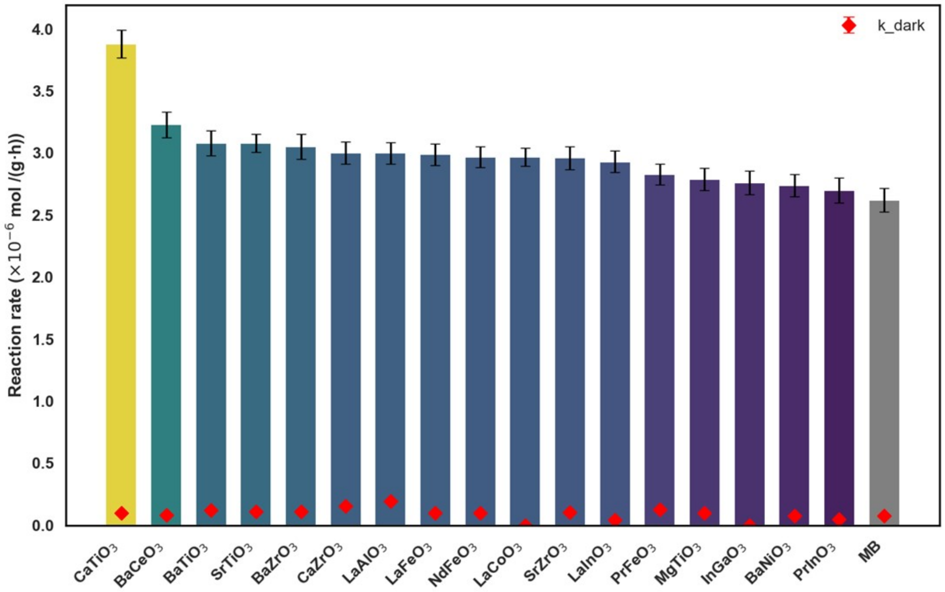

Figure S5: Photocatalytic performance under dark conditions, presented alongside the light-irradiated results from Figure 3. The bar plots represent the performance under light irradiation, while the red dots indicate the corresponding dark-condition results after 24 hours of monitoring. As shown, changes in MB concentration under dark conditions are negligible compared to those under light irradiation.