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ELECTRONIC SUPPORTING INFORMATIONS

Antiferromagnetically Coupled Double Perovskite as an Efficient and Robust Catalyst for Visible Light Driven Water Splitting at Neutral pH

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Table S1: Results of the crystal structure refinements for CFR as obtained from PXRD and neutron powder diffraction.

Refinement parameters	PXRD data	NPD data
T (K)	RT	RT
Space group	*Pnma*	*Pnma*
a [Å]	5.6524(5)	5.6402 (2)
b [Å]	7.9092(7)	7.9077(2)
c [Å]	5.5590(5)	5.5579(2)
V [Å^3]	248.52(4)	247.89(1)
x(Ca/La)	0.0377(2)	0.0418(3)
z(Ca/La)	−0.0055(7)	−0.0099(7)
x(O1)	0.2737(11)	0.2962 (3)
y(O1)	0.0569(8)	0.0461 (3)
z(O1)	0.7112(11)	0.7050 (3)
x(O2)	0.4680(14)	0.4705(4)
y(O2)	0.25	0.25
z(O2)	0.072 (2)	0.0862 (6)
R_F	3.51	1.69
d_{ap}(Fe/Ru-O′1) [Å]	1.9936(62)	2.0353(17)
d_{eq} (Fe/Ru-O1) (Å)	2.101 (62)	2.0548(17)
d_{eq} (Fe/Ru-O2) (Å)	2.0255(23)	2.409(8)

Table S2: Controlled experiments to optimize the photocatalytic performance of CLSR catalyst

Set No.	CFR catalyst	Photosensitizer	Sodium thiosulphate	Observation
1	No	Yes	Yes	No OER
2	Yes	No	Yes	No OER
3	Yes	Yes	No	No OER

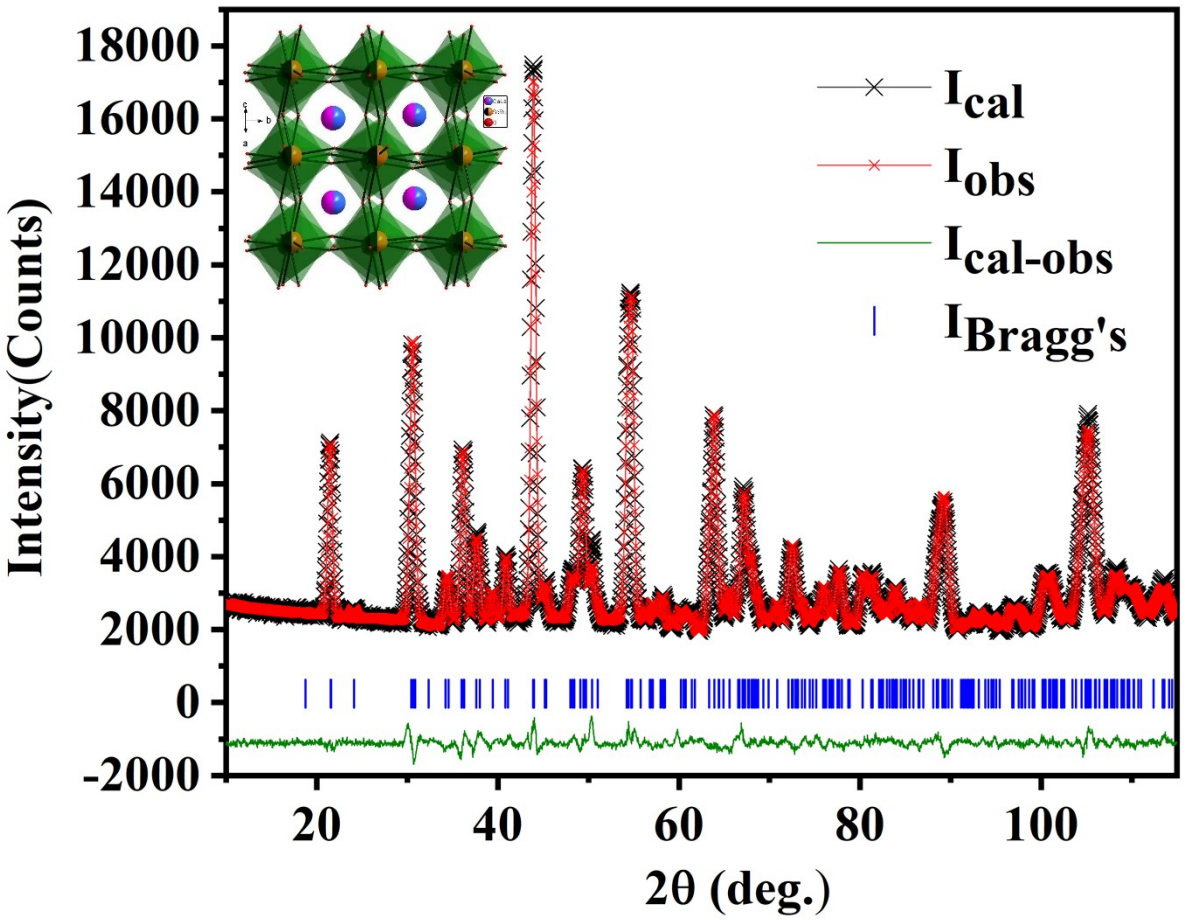

Fig. S1: Rietveld refinement of room temperature neutron powder diffraction (NPD) pattern of CLSR catalyst along with crystal structure.

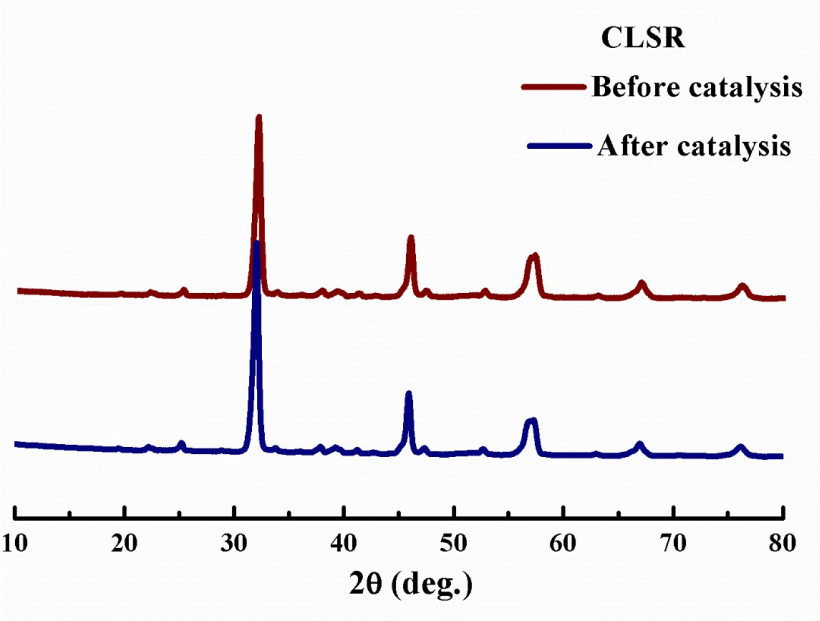

Fig. S2: PXRD of CLSR before and after photocatalytic water oxidation activity.

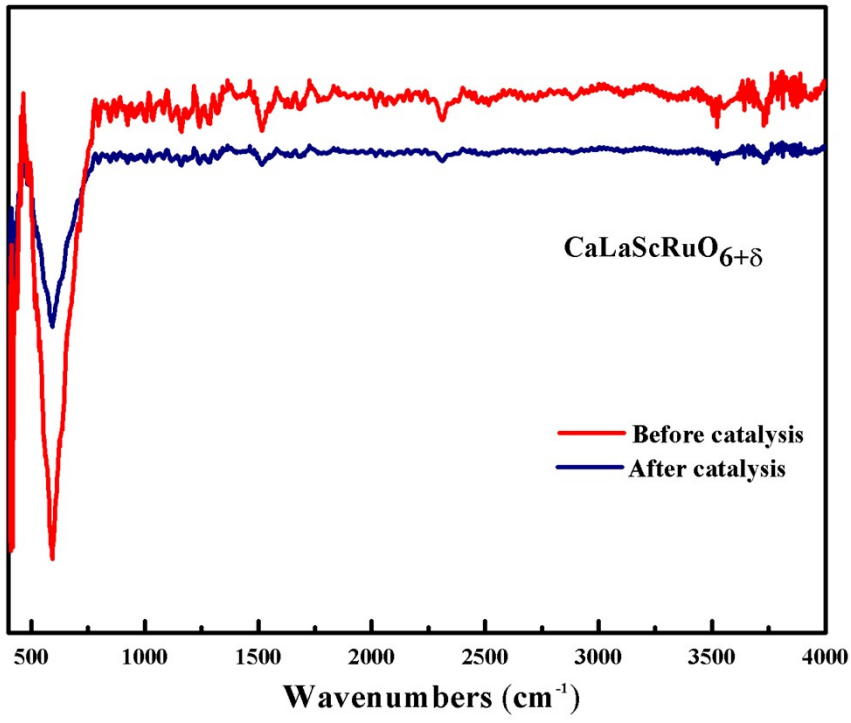

Fig. S3: FT-IR of CLSR before and after photocatalytic water oxidation activity.