

Systematic investigation of ABO₃ perovskite synthesis to generalise a La and Rh co-doping strategy for visible light photocatalysis

Thomas Douglas Small,^[1] Mahmoud Adel Hamza,^{[1], [2]} Yideng Shen,^[1] Cameron J. Shearer, ^[1] * Gregory F. Metha ^[1] *

^[1] Department of Chemistry, University of Adelaide, Adelaide SA 5005, Australia
^[2] Chemistry Department, Faculty of Science, Ain Shams University, Abbassia, Cairo, 11566, Egypt

*Corresponding author: cameron.shearer@adelaide.edu.au, greg.metha@adelaide.edu.au

Supporting Information

Table S1: The theoretical ratios between A, B, and dopants elements and the corresponding actual ratios measured by ICP-MS.

Sample	Theoretical Ratio	Actual ratio
SrZrO ₃	Sr : Zr = 1 : 1	1 : 1.04
La, Rh - SrZrO ₃	Sr : Zr : Rh : La = 1 : 1 : 0.04 : 0.04	1 : 1.09 : 0.0331 : 0.0399
SrZr _{0.5} Ti _{0.5} O ₃	Sr : Zr : Ti = 1 : 0.5 : 0.5	1 : 0.574 : 0.561
La, Rh - SrZr _{0.5} Ti _{0.5} O ₃	Sr : Zr : Ti : Rh : La = 1 : 0.5 : 0.5 : 0.04 : 0.04	1 : 0.579 : 0.568 : 0.00855 : 0.0430
SrTiO ₃	Sr : Ti = 1 : 1	1 : 1.06
La, Rh - SrTiO ₃	Sr : Ti : Rh : La = 1 : 1 : 0.04 : 0.04	1 : 1.07 : 0.0373 : 0.0451
BaZrO ₃	Ba : Zr = 1 : 1	1 : 0.91
La, Rh - BaZrO ₃	Ba : Zr : La : Rh = 1 : 1 : 0.04 : 0.04	1 : 0.95 : 0.0212 : 0.0267
BaZr _{0.5} Ti _{0.5} O ₃	Ba : Zr : Ti = 1 : 0.5 : 0.5	1 : 0.47 : 0.45
La, Rh - BaZr _{0.5} Ti _{0.5} O ₃	Ba : Zr : Ti : La : Rh = 1 : 0.5 : 0.5 : 0.04 : 0.04	1 : 0.50 : 0.48 : 0.0114 : 0.0343
BaTiO ₃	Ba : Ti = 1 : 1	1 : 0.93
La, Rh - BaTiO ₃	Ba : Ti : La : Rh = 1 : 1 : 0.04 : 0.04	1 : 0.90 : 0.0484 : 0.0780

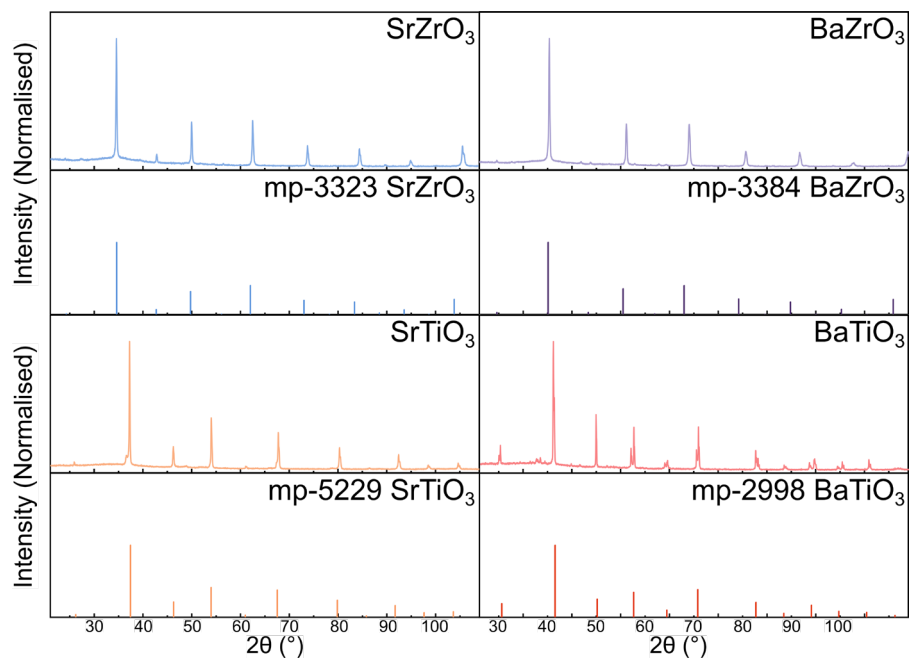


Figure S1: Experimental PXRD traces compared with PXRD traces from the Materials Project

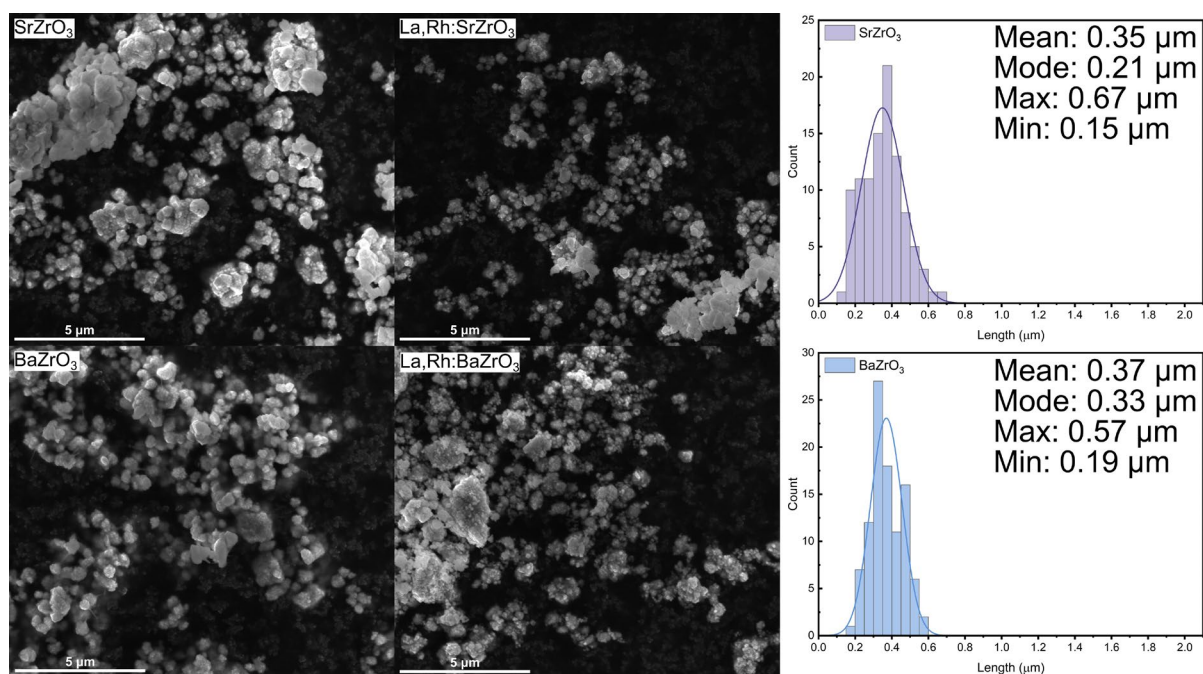


Figure S2: SEM images and particle size histograms of AZrO₃ perovskites

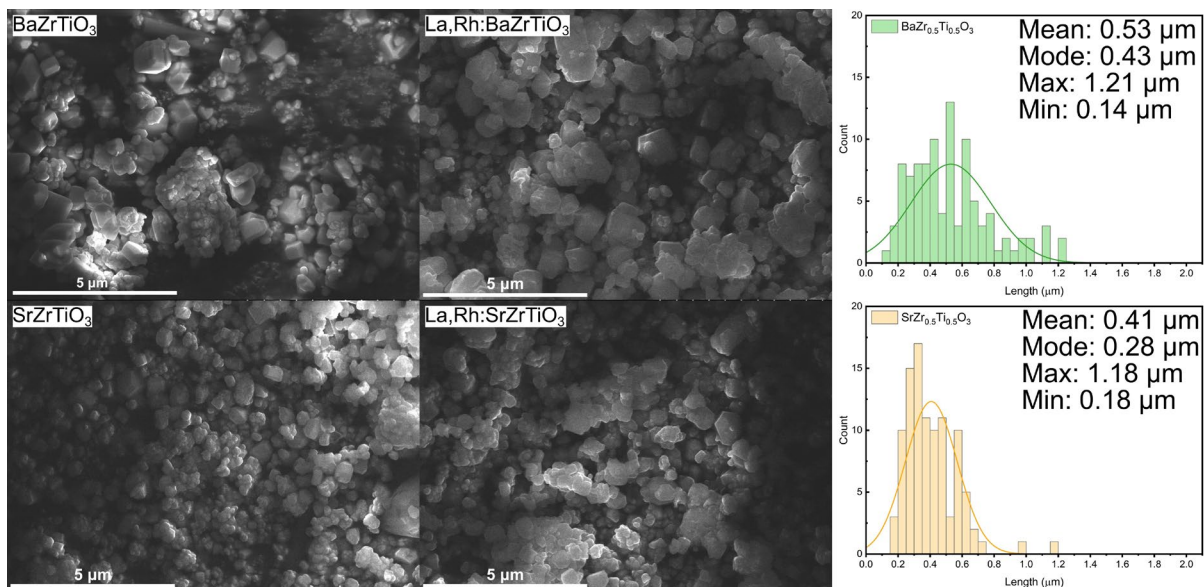


Figure S3: SEM images and particle size histograms of $AZr_{0.5}Ti_{0.5}O_3$ perovskites

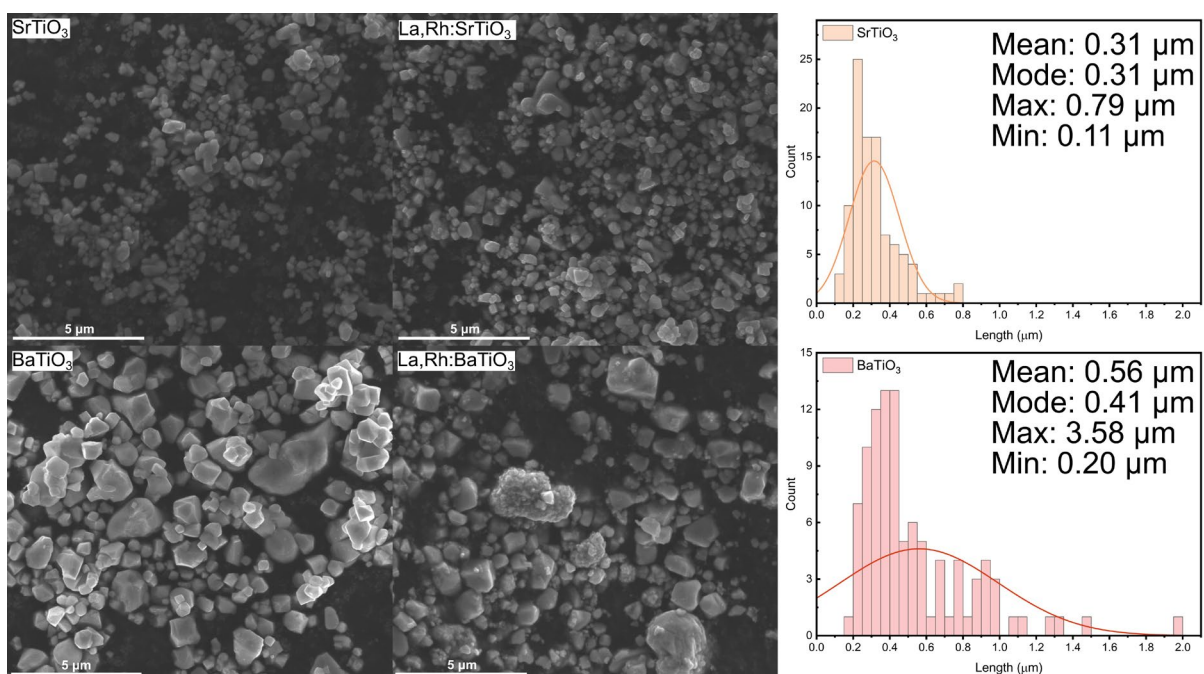
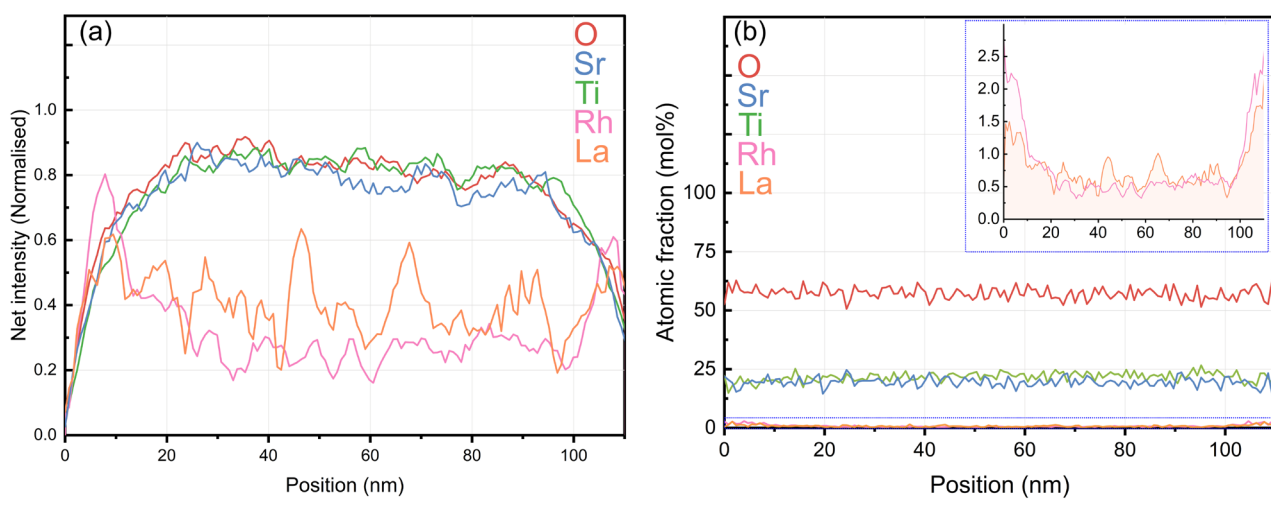


Figure S4: SEM images and particle size histograms of $ATiO_3$ perovskites

25



26

27

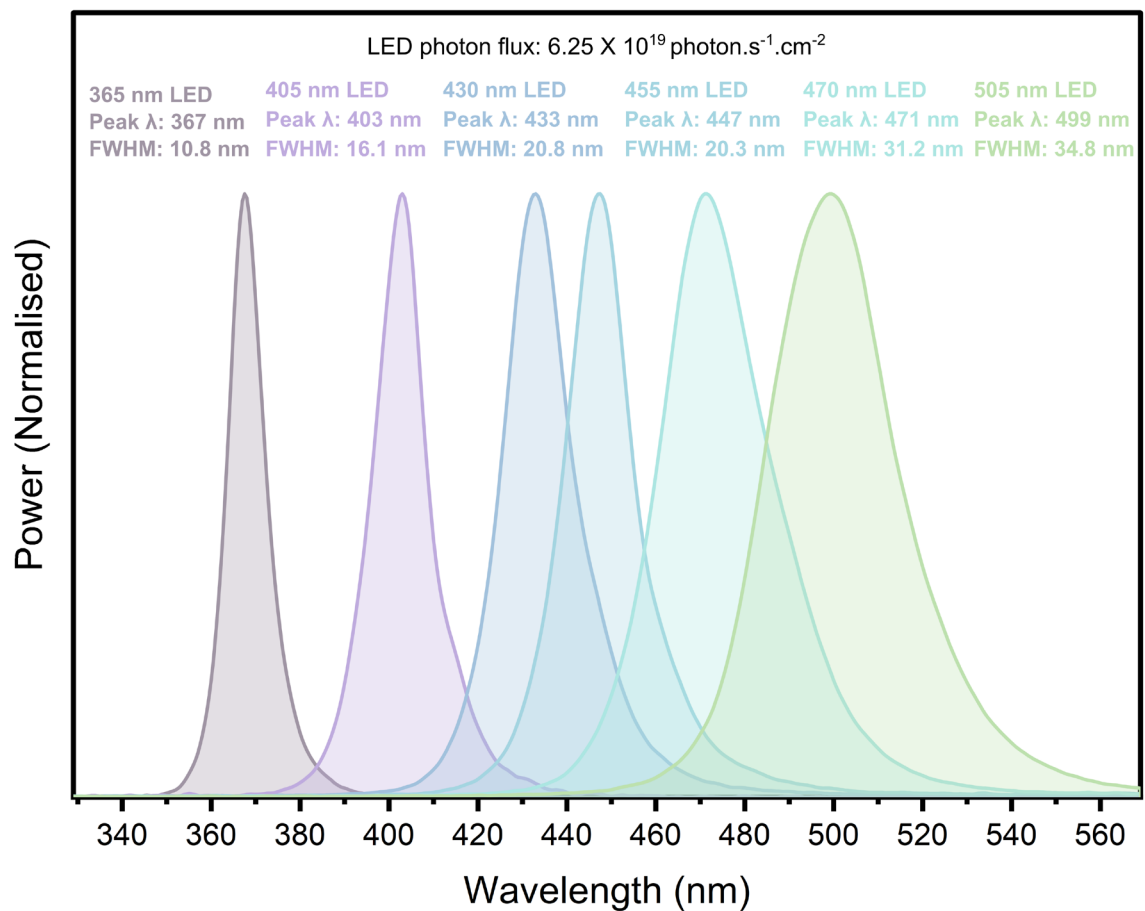
28

29

30

31

Figure S5: (a) EDS line profile of net signal intensity for O, Sr, Ti, Rh and La across the arrow in Figure 7b. A moving average (data window = 5) was applied to average the data over multiple lines. (b) EDS line profile of atomic fraction for O, Sr, Ti, Rh and La across the arrow in Figure 7b. The inset depicts an enlarged view of graph with reduced y-axis range.



32

33

Figure S6: Spectral power distributions of 365, 405, 430, 455, 470 and 505 nm LEDs.

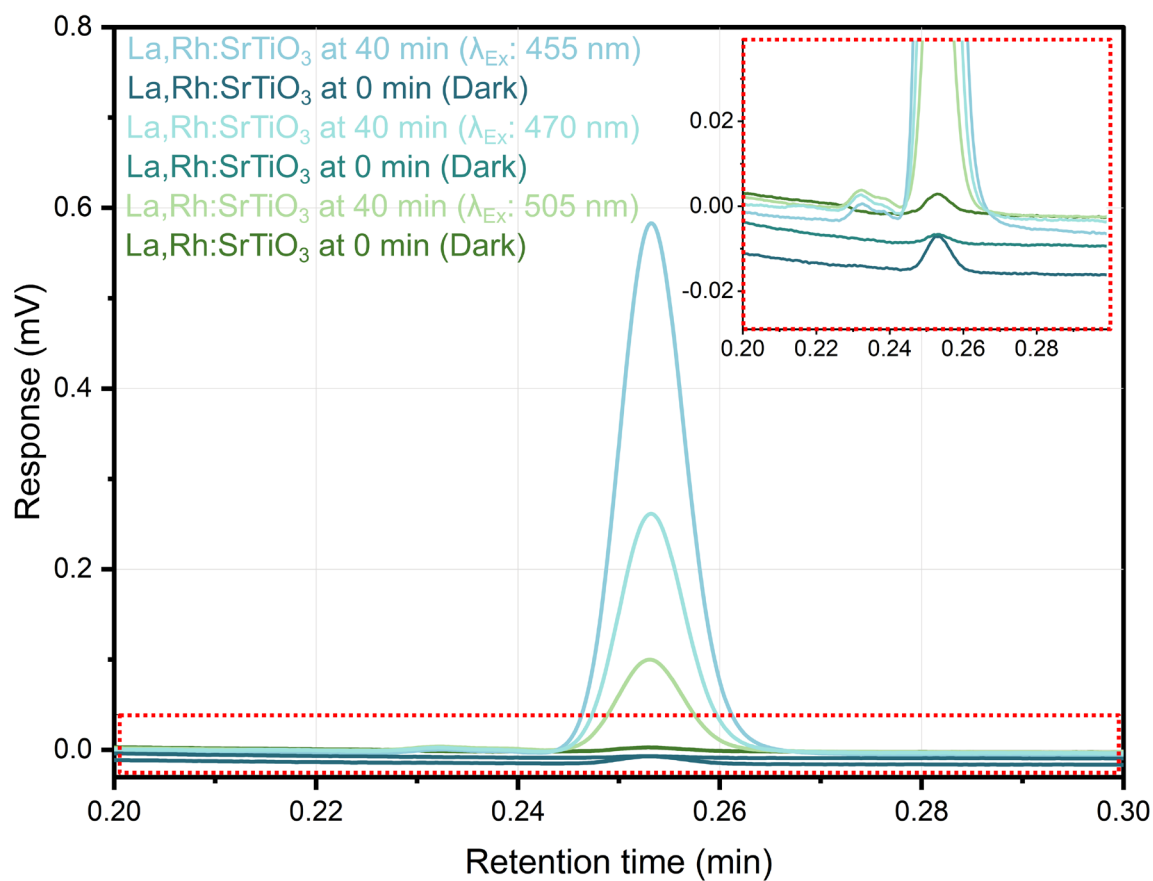


Figure S7: Gas chromatographs of the H₂ peak obtained under dark conditions and after 40 min of illumination excitation wavelengths of 455, 470 and 505 nm. The vertical axis in the inset is truncated to aid visualisation of the peaks obtained with the dark condition.