Electronic supplementary information

$LaTiO_2N$-$LaCrO_3$: continuous solid solutions towards enhanced photocatalytic H_2 evolution under visible-light irradiation

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Calculation of the tolerance factor

Goldschmidt proposed the tolerance factor (t) for ABX_3-type perovskites,[1]

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)} \qquad (S1)$$

in which r_A, r_B, and r_X are the ionic radii of A, B and X located in 12-, 6-, and (2 + 4)-fold coordinated environments, respectively. In the case of complex perovskites, in which more than one ion occupies the A, B and/or X sites, the average radius of the ions on each site is used for r_A and r_B, respectively. Herein, the Shannon effective ionic radii (in pm) of related ions were employed as follows:[2] La^{3+}: 136 (12) for A-site occupancy; Ti^{4+}: 60.5 (6) and Cr^{3+}: 61.5 (6) for B-site occupancy; O^{2-}: 140 (6) and N^{3-}: 150 (6) for X-site occupancy. Data in brackets are coordination numbers (CN). Consequently, The t values of $LaTiO_2N$, $(LaTiO_2N)_{0.9}(LaCrO_3)_{0.1}$ (i.e., $LaTi_{0.9}Cr_{0.1}O_{2.1}N_{0.9}$), $(LaTiO_2N)_{0.8}(LaCrO_3)_{0.2}$ (i.e., $LaTi_{0.8}Cr_{0.2}O_{2.2}N_{0.8}$), $(LaTiO_2N)_{0.7}(LaCrO_3)_{0.3}$ (i.e., $LaTi_{0.7}Cr_{0.3}O_{2.3}N_{0.7}$), $(LaTiO_2N)_{0.6}(LaCrO_3)_{0.4}$ (i.e., $LaTi_{0.6}Cr_{0.4}O_{2.4}N_{0.6}$), $(LaTiO_2N)_{0.4}(LaCrO_3)_{0.6}$ (i.e., $LaTi_{0.4}Cr_{0.6}O_{2.6}N_{0.4}$) and $LaCrO_3$ were calculated to be 0.96902, 0.96897, 0.96893, 0.96888, 0.96883, 0.96874 and 0.96854, respectively.

Notes and references

1. V. M. Goldschmidt, *Naturwissenschaften*, 1926, **14**, 477-485.

2. R. D. Shannon, *Acta Crystallographica Section A*, 1976, **32**, 751-767.

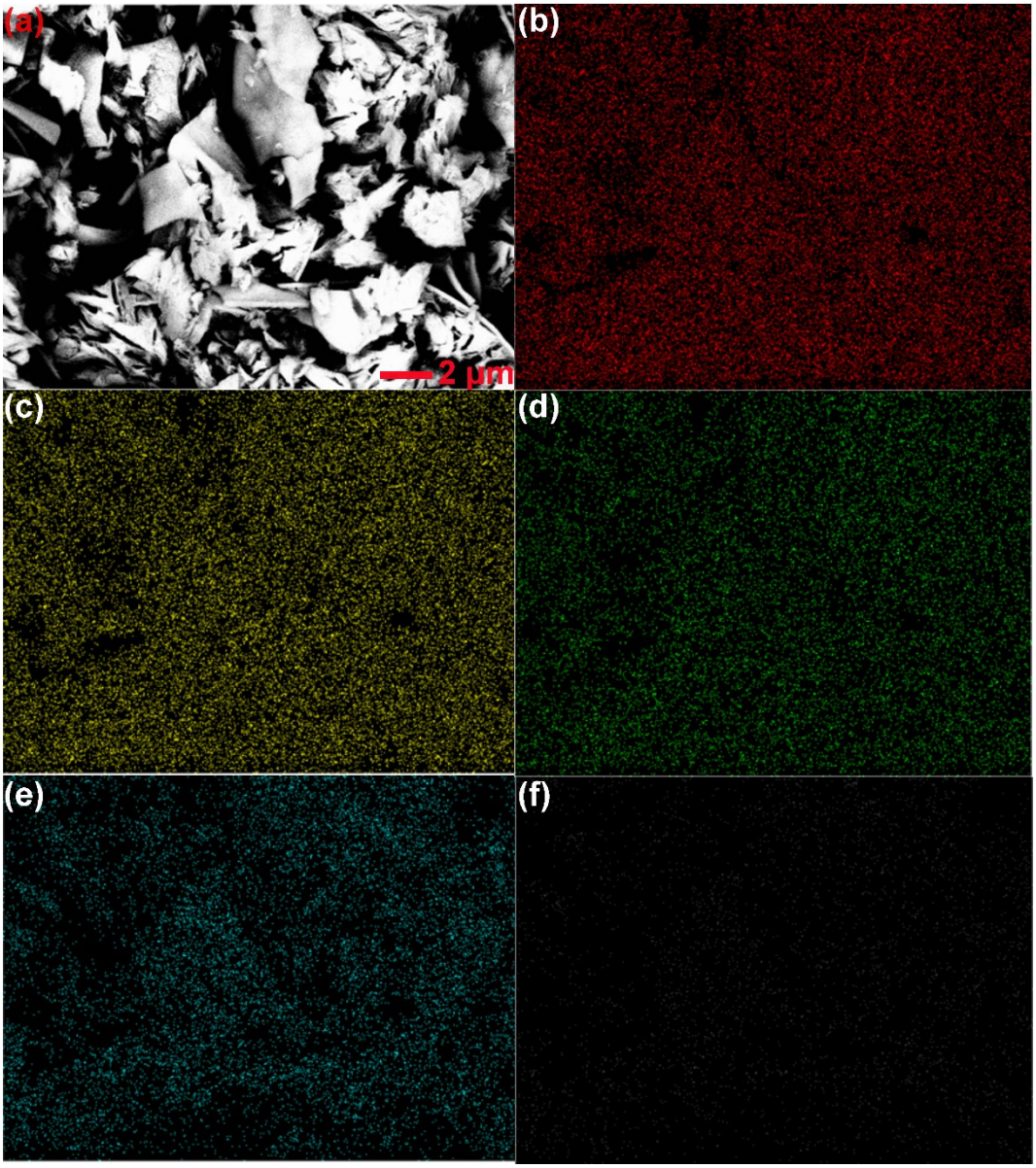

Fig. S1. (a) SEM image and (b-f) elemental mapping images of (b) La, (c) Ti, (d) Cr, (e) O and (f) N for LTON-0.3LCO. Scale bar: 2 μm.

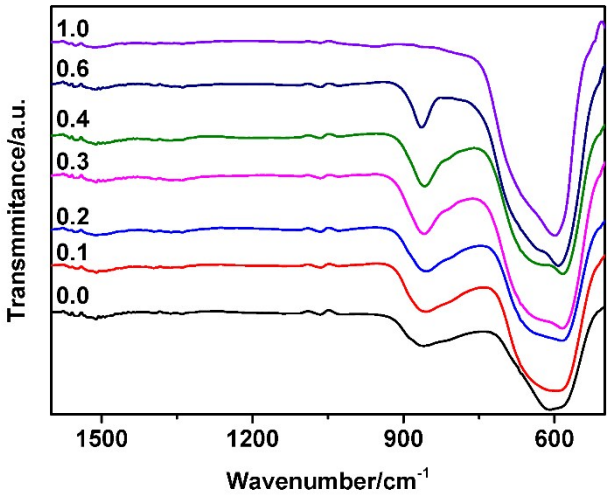

Fig. S2. FTIR spectra for LTON-*x*LCO samples (*x* = 0.0, 0.1, 0.2, 0.3, 0.4, 0.6 and 1.0) in the range from 1600 to 500 cm^{-1}.

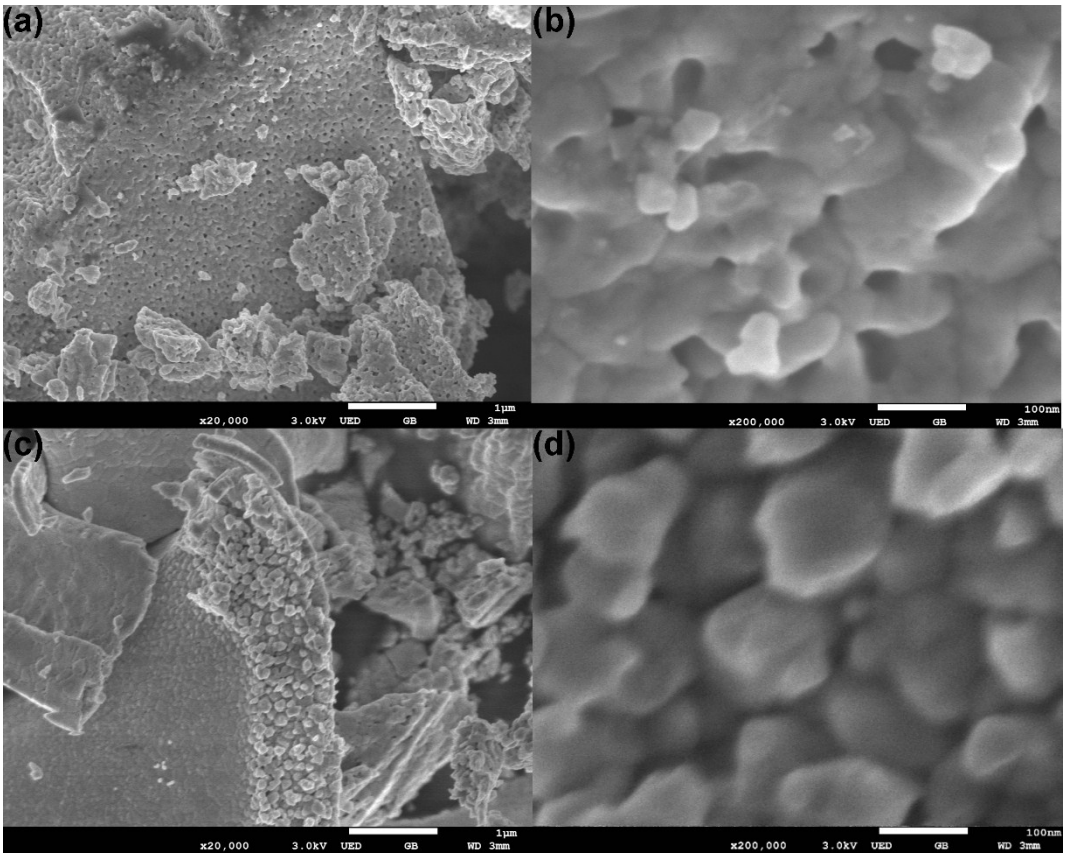

Fig. S3. SEM images for LTON-*x*LCO samples with *x* = (a, b) 0.1, and (c, d) 0.6. Scale bar: (a, c) 1 μm, (b, d) 100 nm.

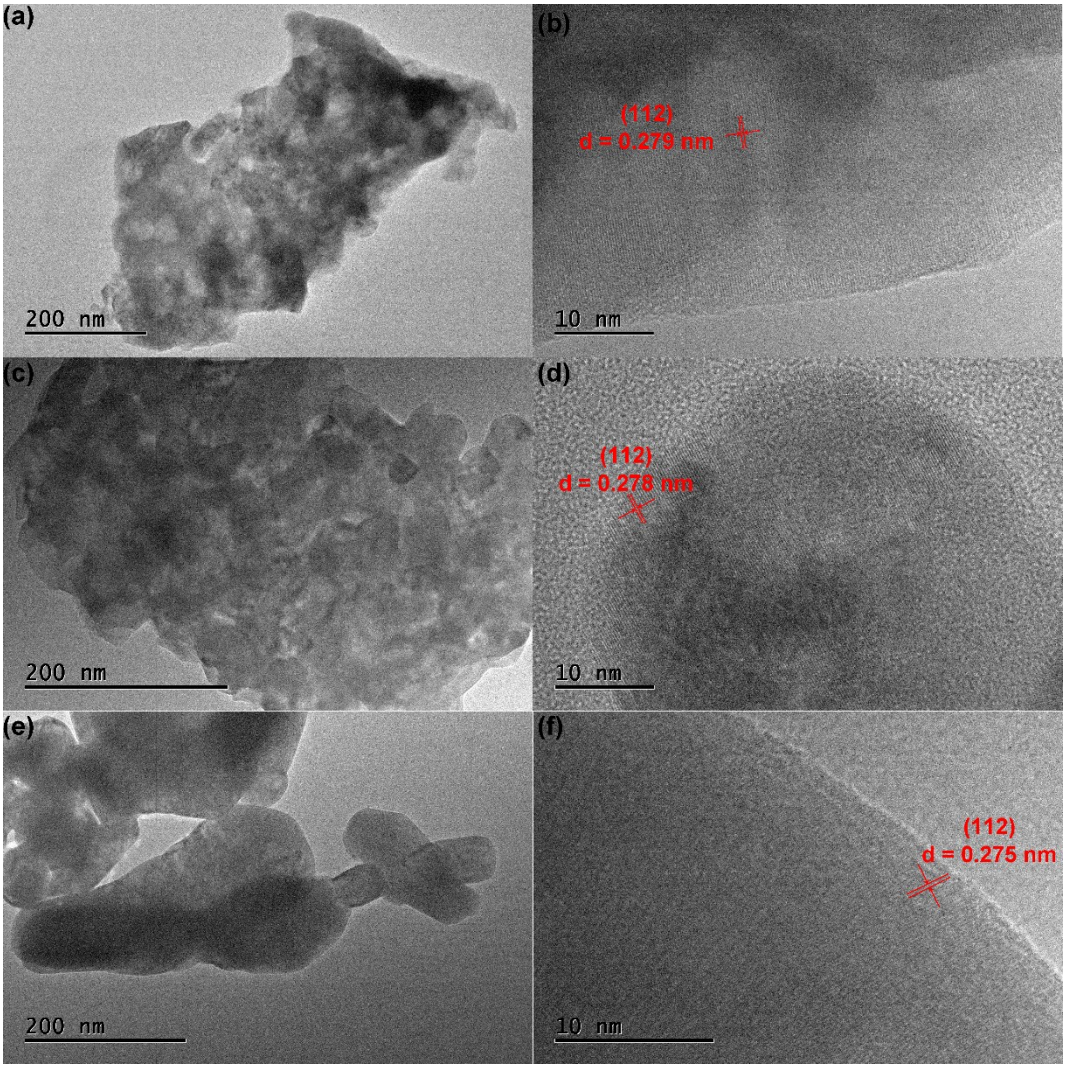

Fig. S4. (a, c, e) TEM and (b, d, f) HRTEM images for LTON-*x*LCO samples with *x* = (a, b) 0.0, (c, d) 0.3, and (e, f) 1.0. Scale bar: (a, c, e) 200 nm, (b, d, f) 10 nm.

Table S1. Binding energies (unit: eV) of Cr 2p and N 1s levels for LTON-*x*LCO samples (*x* = 0.0, 0.1, 0.2, 0.3, 0.4, 0.6 and 1.0).

Sample	Cr				N
	$2p_{3/2}$		$2p_{1/2}$		1s
LTON-0.0LCO	-[a]	-[a]	-[a]	-[a]	395.3
LTON-0.1LCO	575.3	578.4	585.2	589.7	395.3
LTON-0.2LCO	575.9	578.5	585.5	589.1	395.4
LTON-0.3LCO	576.0	579.1	585.6	588.2	395.4
LTON-0.4LCO	576.0	578.6	585.6	588.2	395.5
LTON-0.6LCO	576.3	579.0	585.8	588.7	395.5
LTON-1.0LCO	576.0	578.2	585.7	587.8	-[a]

[a] Not detected.