Supporting Information (SI):

Water splitting cycle for hydrogen production at photo-induced oxygen vacancies using solar energy: experiments and DFT calculation on pure and metal-doped CeO_2

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Including 13 Figures, 2 Tables.

1. Lists of materials for fabrication

CeO_2 purchased from Aladdin (Ar, 99.5%).

Iron (III) nitrate nonahydrate ($Fe(NO_3)_3$) purchased from Macklin (Ar, 99%).

Cerium nitrate hexahydrate ($Ce(NO_3)_3$) purchased from Macklin (Ar, 99%).

Chromium (III) nitrate nonahydrate ($Cr(NO_3)_3$) purchased from Aladdin (Ar, 98.5%).

Cobalt nitrate hexahydrate ($Co(NO_3)_2$) from Aladdin (Ar, 99%).

Zirconium (IV) oxynitrate hydrate ($Zr(NO_3)_2$) from Aladdin (Ar, 99.5%).

Zinc nitrate hexahydrate ($Zn(NO_3)_2$) from Aladdin (Ar, 99%).

Copper nitrate hydrate ($Cu(NO_3)_2$) from Aladdin (Ar, 99%).

Samarium(III) nitrate hexahydrate ($Sm(NO_3)_3$) from chronchem (Ar, 99%).

Lanthanum nitrate hexahydrate ($La(NO_3)_3$) from Aladdin (Ar, 99%).

Neodymium nitrate hexahydrate ($Nd(NO_3)_3$) from chronchem (Ar,9 9%).

Table S1. The experimental and calculated doping ratio

Doped element	Calculated ratio (%)	Experimental ratio (%)
Sm	10	9.5
Nd	10	7.9
La	10	10.6
Zn	10	11.8
Zr	10	10.7
Cu	10	9.7
Fe	10	8.0
Cr	10	10.8
Co	10	9.9

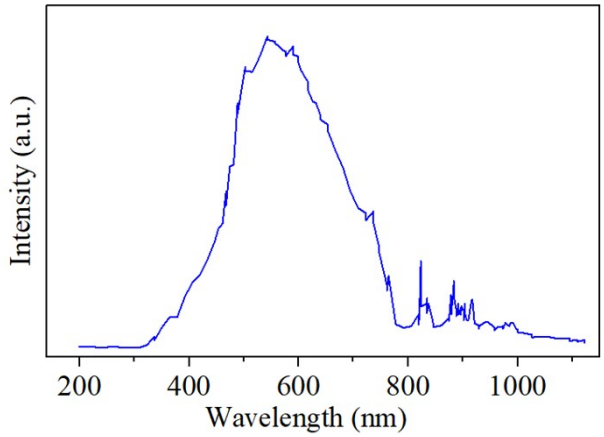

Fig. S1. Spectrum of 300W Xenon lamp.

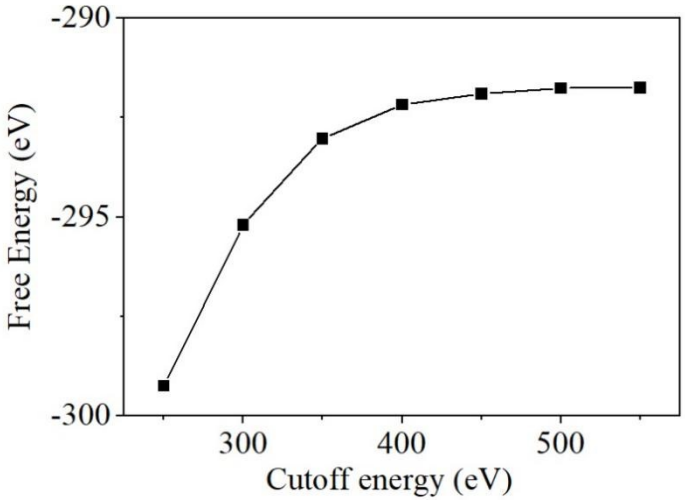

Fig. S2. Correlation between free energy and cutoff energy

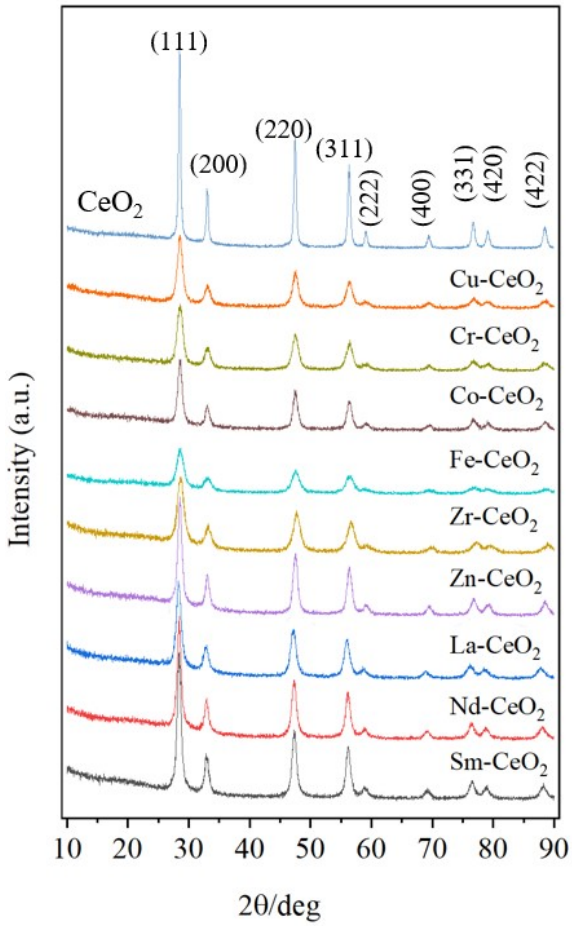

Fig. S3. XRD patterns of pure CeO_2 and metal-doped CeO_2.

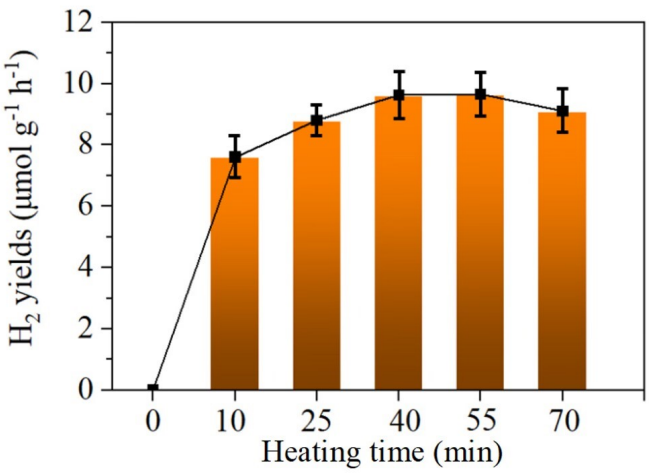

Fig. S4. H_2 yields by CeO_2 in individual PTC experiments with different heating time.

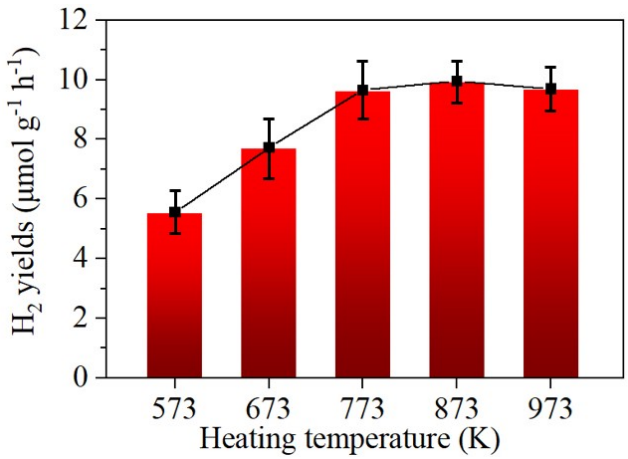

Fig. S5. H_2 yields by CeO_2 in individual PTC experiments with different heating temperature.

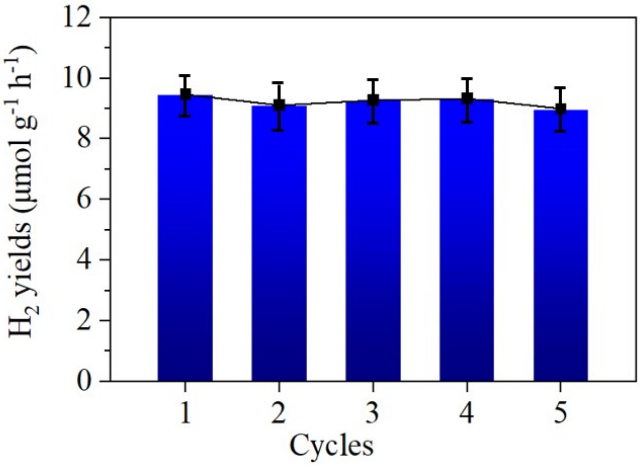

Fig. S6. H_2 yields by CeO_2 in five consecutive cycles of the PTC experiments (irradiation time: 40 min, heating time: 40 min, heating temperature: 773 K).

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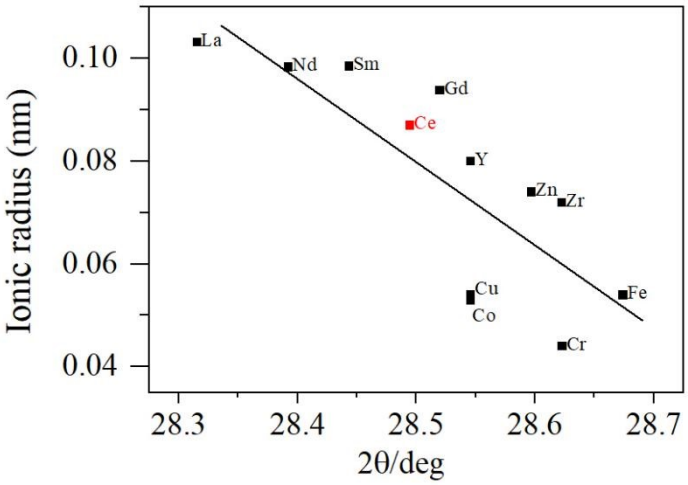

Fig. S7. The relationship between the (111) plane shifts and the ion radius of dopants.

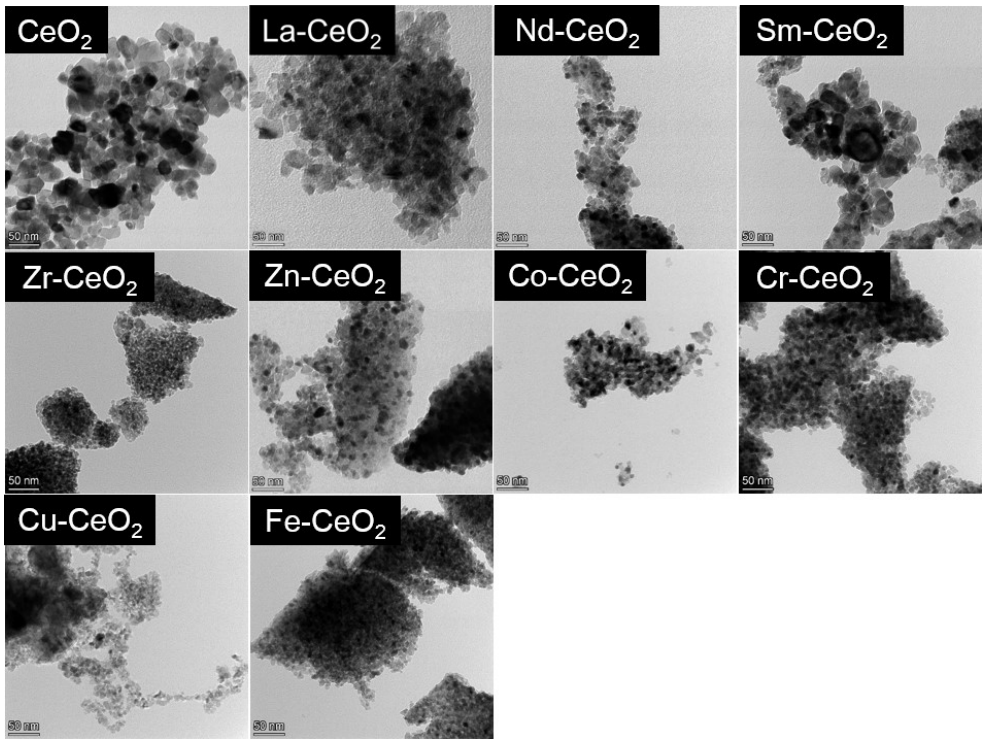

Fig. S8. TEM images of pure CeO_2 and metal-doped CeO_2.

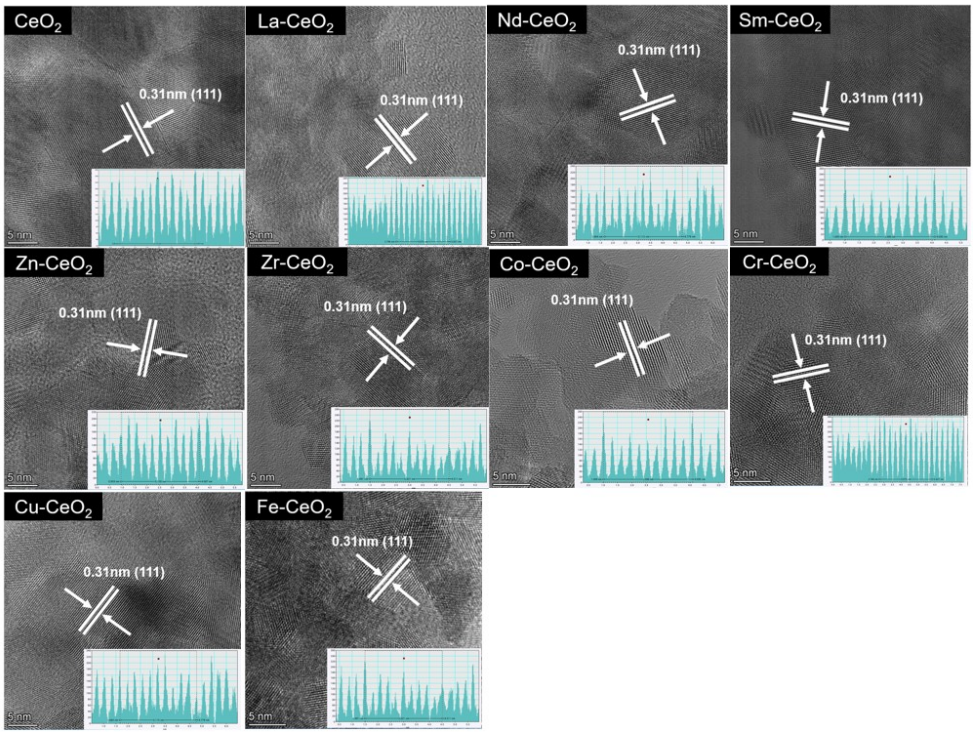

Fig. S9. TEM images of pure CeO_2 and metal ions doped CeO_2.

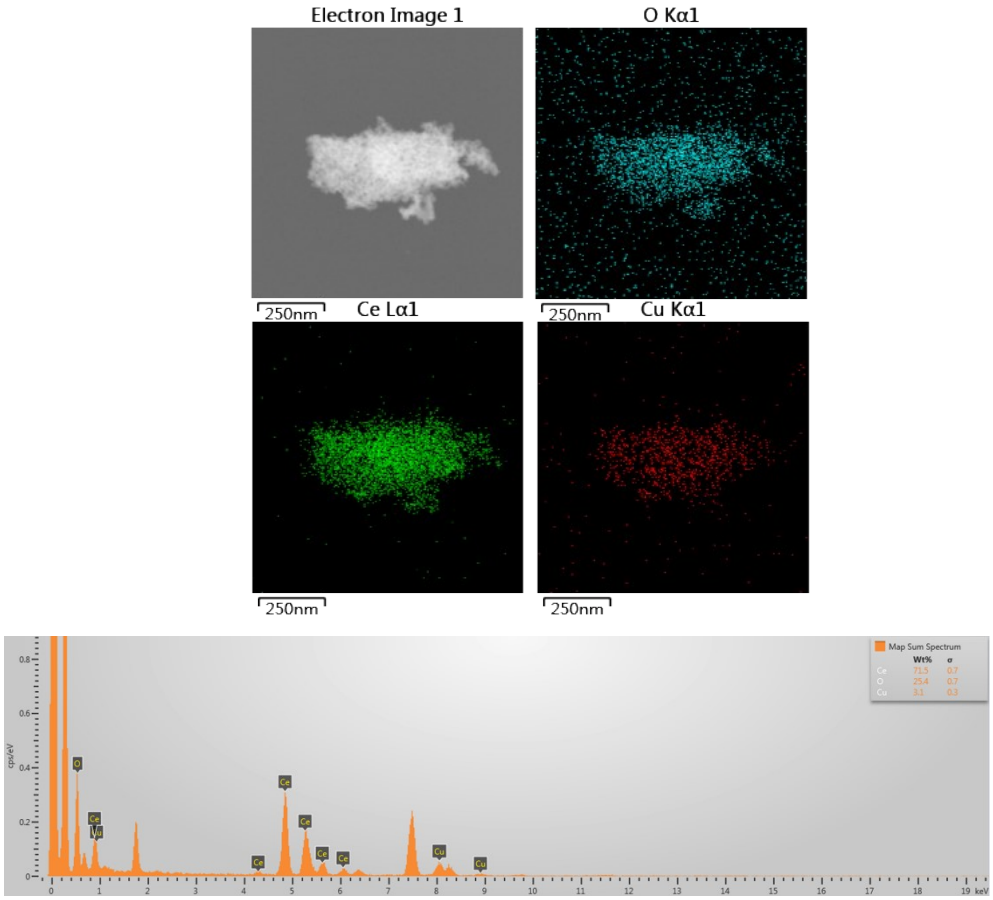

Fig. S10. EDS mapping of Cu-CeO_2.

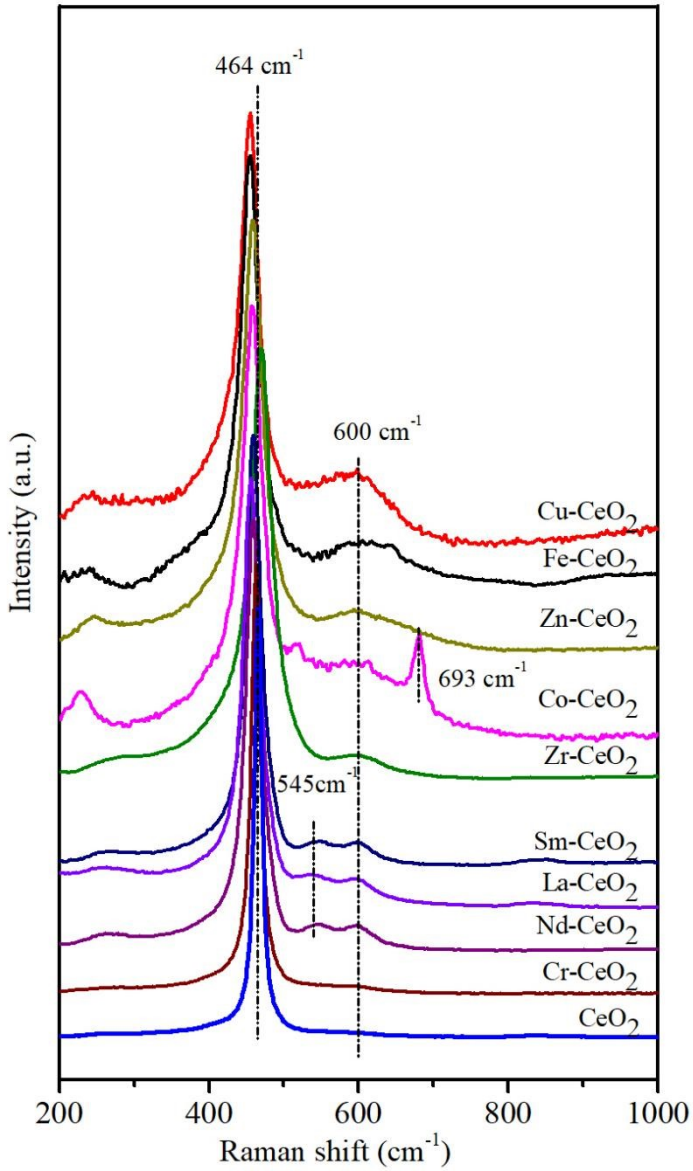

Fig. S11. Raman spectra of CeO_2 and metal ions doped CeO_2.

Table S2. The element ratio of Cu-TiO_2 obtained by EDS

Elements	Wt%	At%
O	25.1	73.31
Cu	3.86	2.81
Ce	71.5	23.86

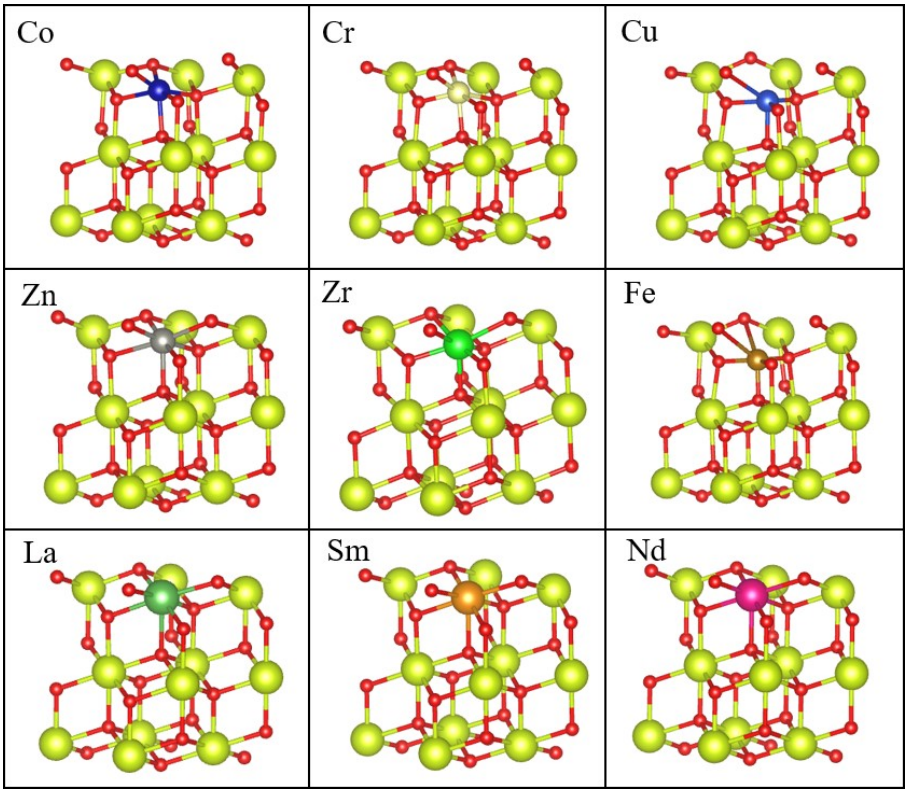

Fig. S12. Models of metal-doped CeO_2 presenting lattice distortion.

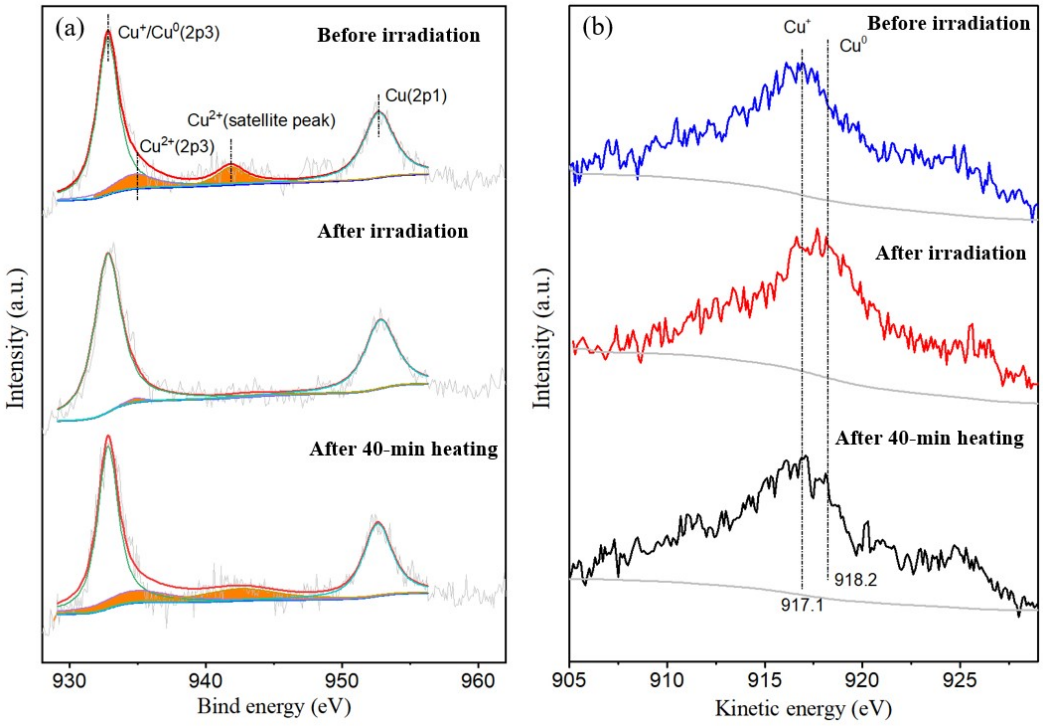

Fig. S13. (a) Cu-2p XPS spectra of the Cu-CeO_2; (b) Auger spectra of Cu LMM.