Electronic Supplementary Material (ESI) for Nanoscale.
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Supporting information

Synergistic effect of atomically dispersed Cu species and Ti-defects for boosting photocatalytic CO_2 reduction over hierarchical TiO_2

Peijiao Chen, Zhijun Li*, Pengze Wang, Yuxin Yao, Tianwei Dou, Yang Qu, Liqiang Jing

Key Laboratory of Functional Inorganic Materials Chemistry (Ministry of Education), School of Chemistry and Materials Science, International Joint Research Center for Catalytic Technology, Heilongjiang University, Harbin 150080, P. R. China.

e-mail address: 2018011@hlju.edu.cn

Computational Methods.

DFT calculations were performed using the Vienna *ab initio* simulation package (VASP). Projector augmented wave potentials were used to describe the interaction of ionic cores and electrons, in the framework of Perdew-Burke-Ernzerhof exchange-correlation density functional[1]. All the calculations were performed with a plane-wave cutoff of 480 eV using 2*2*2 k-point mesh. The force convergence criterion used for geometry relaxations was 0.02 eV/Å.

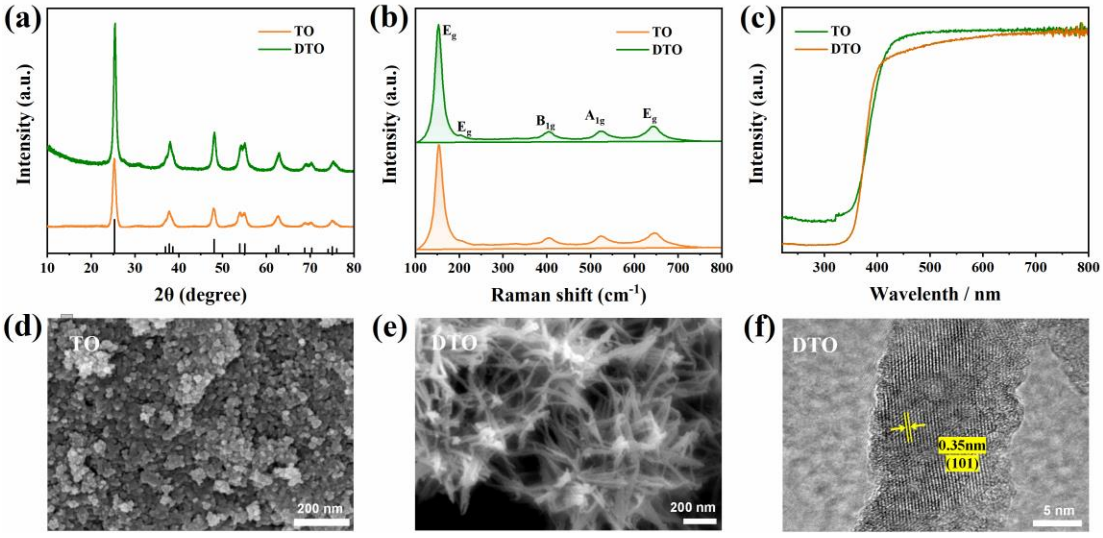

Fig. S1. (a) XRD patterns, (b) Raman spectra, (c) DRS of TO and DTO, SEM images of TO (d) and DTO (e), (f) HR-TEM image of DTO.

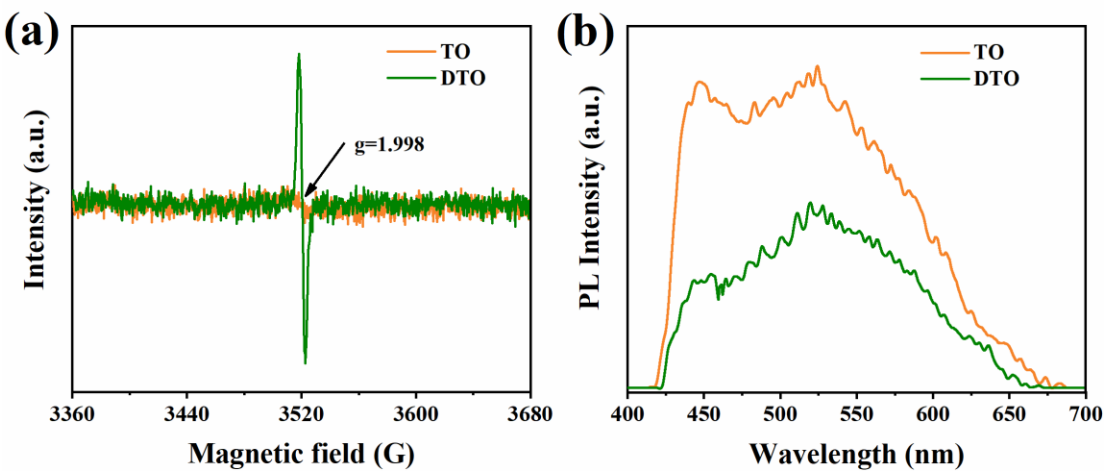

Fig. S2. (a) X-band EPR and (b) PL spectra of TO and DTO.

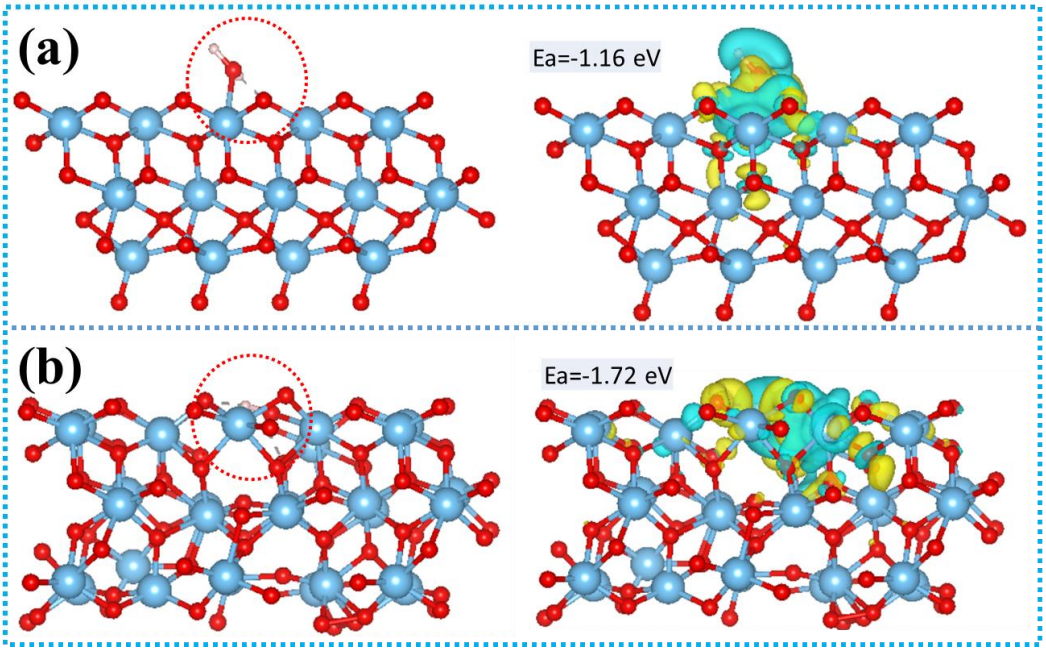

Fig. S3. Calculated structure models and charge density difference of TiO_2 (101) surface without defects (a) and with Ti-defects (b).

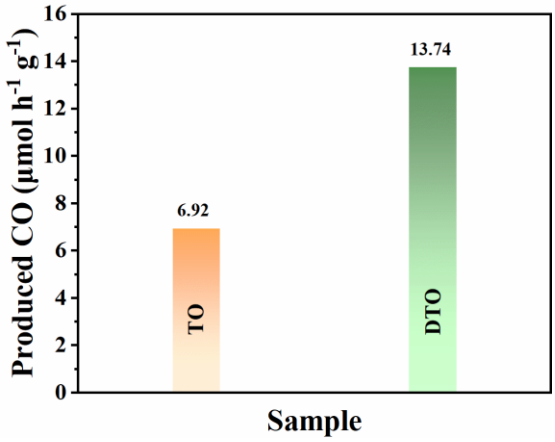

Fig. S4. Photocatalytic performance of TO and DTO for CO_2 reduction under light irradiation.

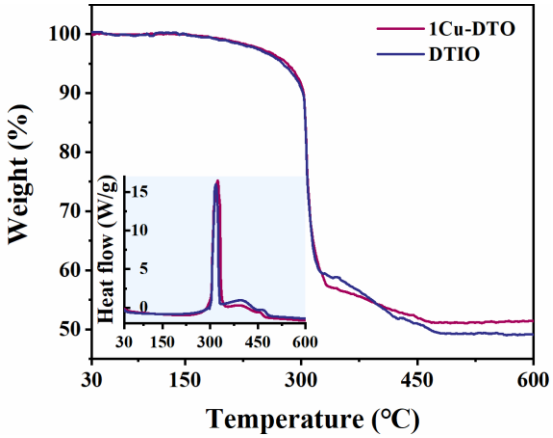

Fig. S5. TG and DTA profiles of intermediate powders of DTO and 1Cu-DTO produced by solvothermal process.

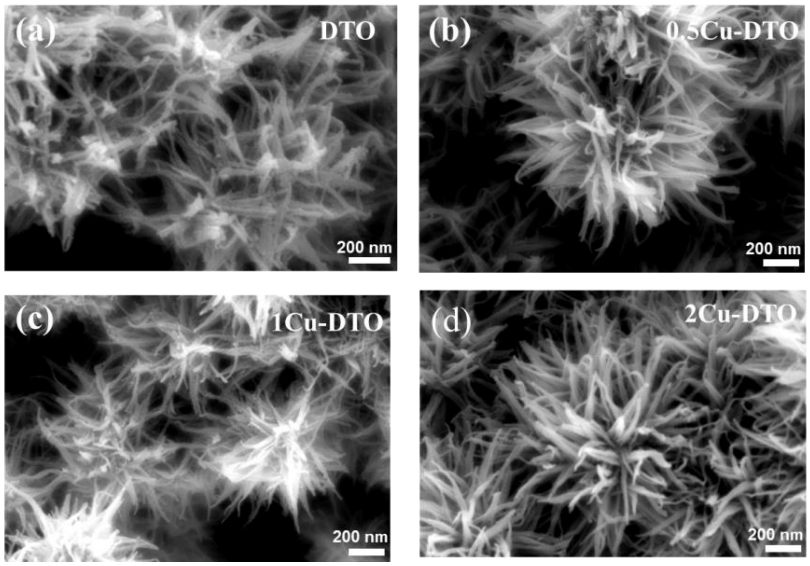

Fig. S6. SEM images of DTO and xCu-DTO.

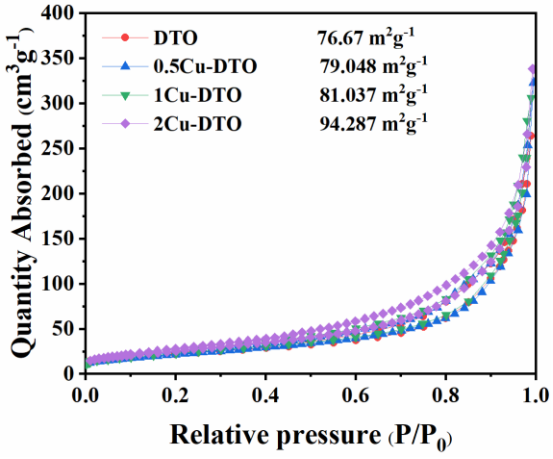

Fig. S7. N_2 adsorption/desorption isotherms of DTO and xCu-DTO.

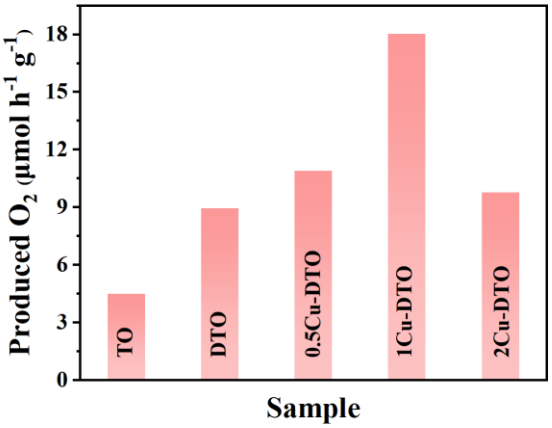

Fig. S8. Photocatalytic performance of TO, DTO and xCu-DTO samples for O_2 generation under light irradiation.

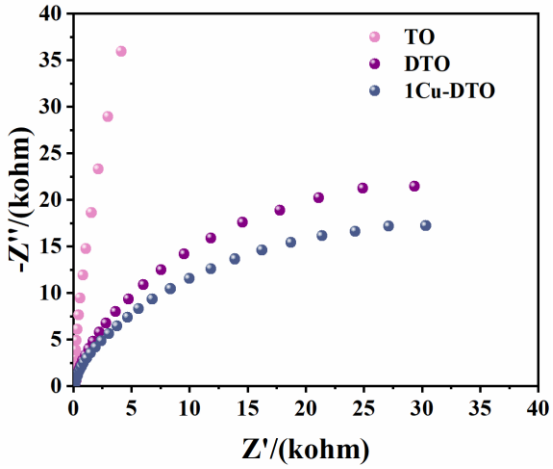

Fig. S9. Electrochemical Impedance Spectroscopy of TO, DTO and 1Cu-DTO.

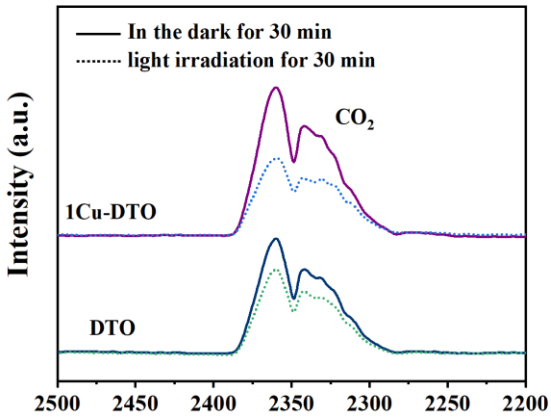

Fig. S10. In-situ FTIR spectra of the adsorbed CO_2 over DTO and 1Cu-DTO before and after light irradiation.

References

1 J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.* , 1996, **77**, 3865-3868.