Supporting Information

Nitrogen and sulfur co-doping CeO_2 nanorods for efficient photocatalytic VOCs degradation

Hui Yang[a, c], Lu Jia[a], Jun Haraguchi[c], Yue Wang[a], Bin Xu[a, *], Qitao Zhang[b, *], Zhaodong Nan[a], Ming Zhang[a], Teruhisa Ohno[c, *]

[a] School of Chemistry and Chemical Engineering, Yangzhou University, Yangzhou 225002, China

[b] International Collaborative Laboratory of 2D Materials for Optoelectronics Science and Technology of Ministry of Education, Institute of Microscale Optoelectronics, Shenzhen University, Shenzhen 518060, China

[c] Department of Applied Chemistry, Faculty of Engineering, Kyushu Institute of Technology, Kitakyushu 804-8550, Japan

***Corresponding authors: twt@yzu.edu.cn (Bin Xu); qitao-zhang@szu.edu.cn (Qitao Zhang); tohno@che.kyutech.ac.jp (Teruhisa Ohno)**

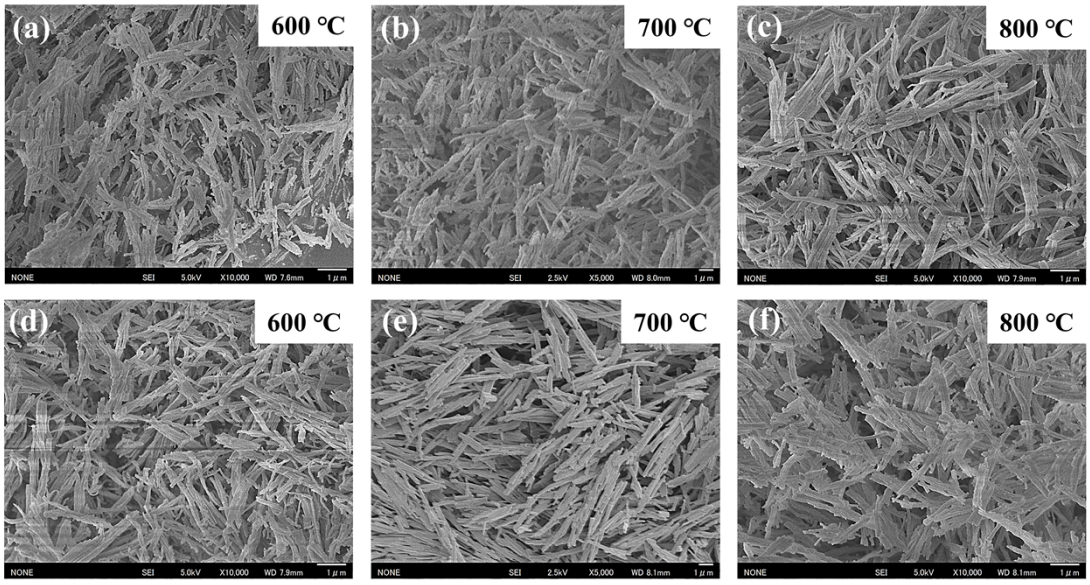

Figure S1. FE-SEM images of (a-c) undoped CeO_2 and (d-f) NS-CeO_2 samples annealed under different temperature conditions, respectively.

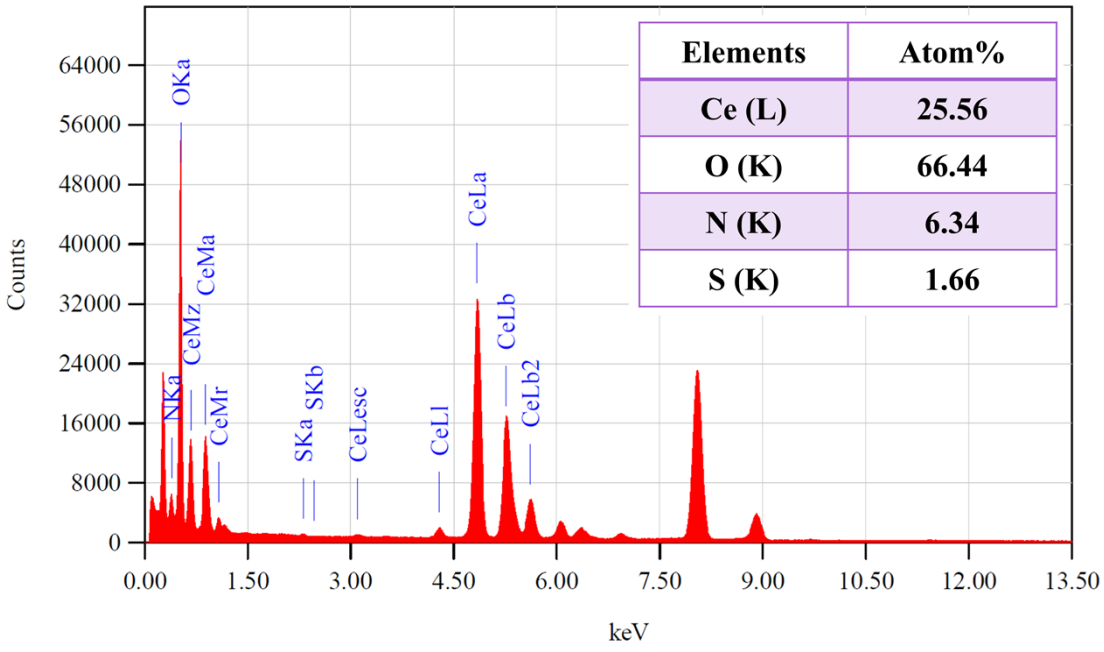

Figure S2. Selected area EDS spectrum of NS-CeO_2 sample annealed at 700°C condition.

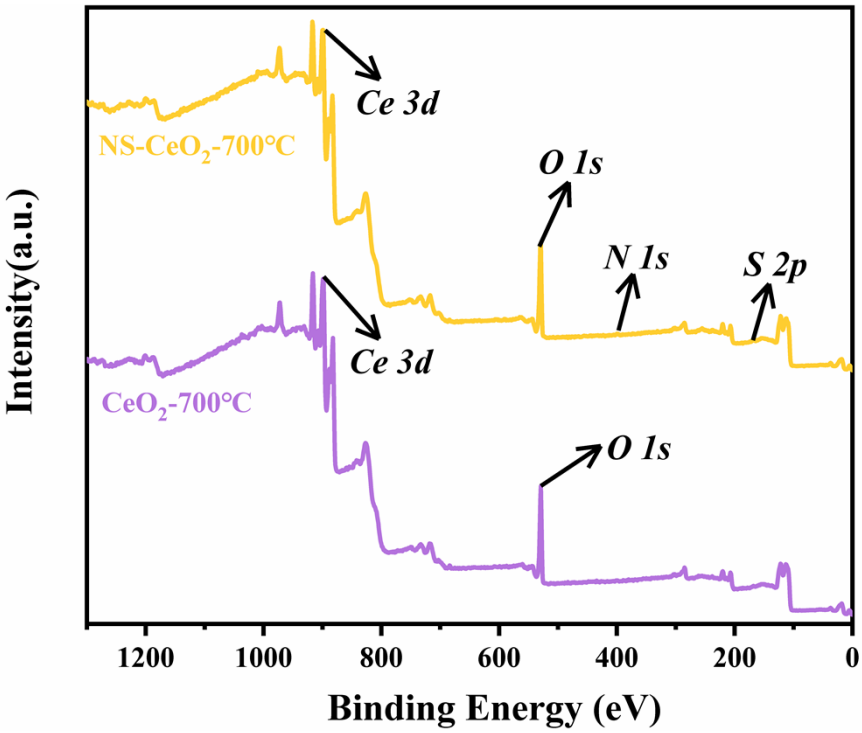

Figure S3. Wide scanning XPS survey spectra of undoped CeO_2 and NS-CeO_2 samples annealed at 700℃ condition.

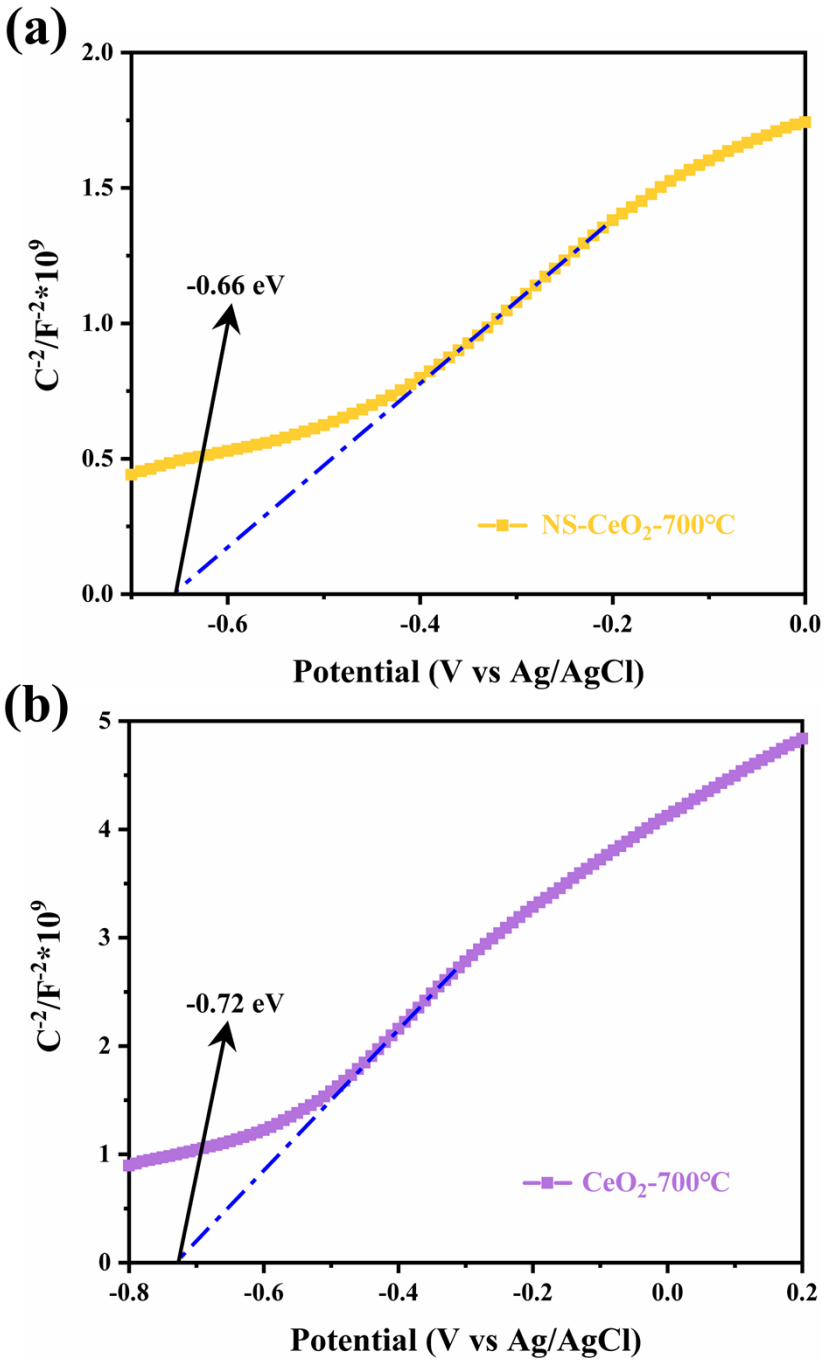

Figure S4. Mott-Schottky (M-S) plots of undoped CeO_2 and NS-CeO_2 samples annealed at 700°C condition.

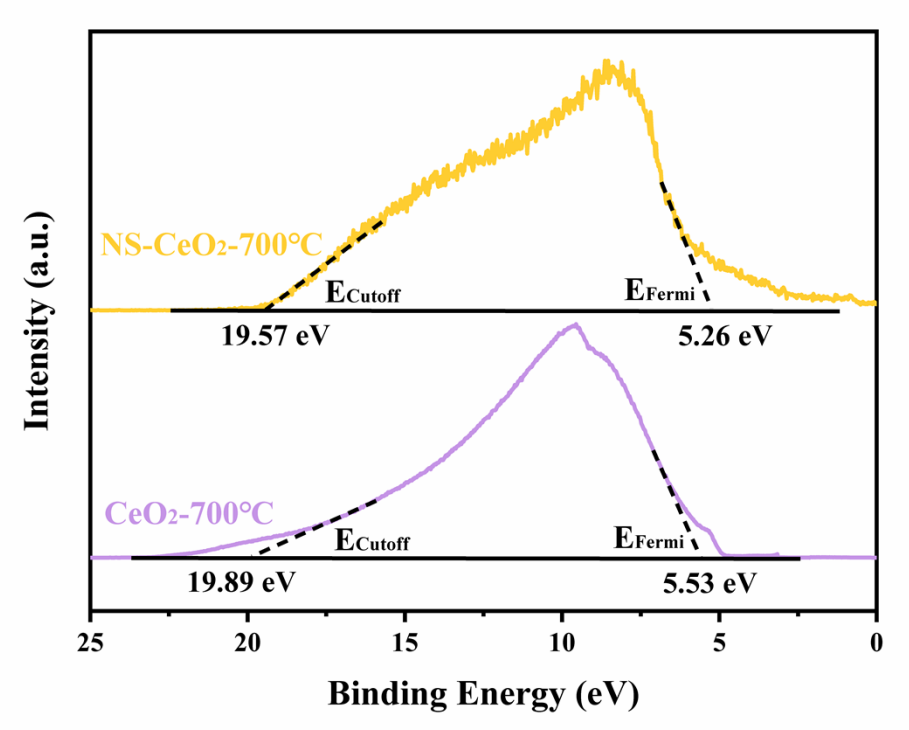

Figure S5. Ultraviolet photoelectron spectroscopy (UPS) signals of NS-CeO_2 and undoped CeO_2 samples annealed at 700℃ condition.

According to the linear intersection method, the valence band (E_{VB}) of NS-CeO_2 was calculated to be 6.91 eV (vs. vacuum) from (E_{Photo} - (E_{Cutoff} - E_{Fermi}) (E_{Photo} = 21.22 eV, the excitation energy of the He I). According to the reference standard of the electron volts convert to electrochemical energy potentials in volts, 0 V versus RHE (reversible hydrogen electrode) corresponding to -4.44 eV versus evac (vacuum level). Then combined with the bandgap value calculated from Tauc plot analysis of NS-CeO_2 (E_g = 2.98 eV), the corresponding conduction band (CB) value is further calculated by the equation $E_{CB} = E_{VB} - E_g$. Thus, the VB and CB positions of NS-CeO_2 are calculated to 2.47 and -0.51 eV, respectively. Notably, these values are very close to that currently obtained from band gap Tauc's plot and Mott-Schottky (M-S) plots (E_{VB} = 2.42 eV, E_{VB} = -0.56 eV).

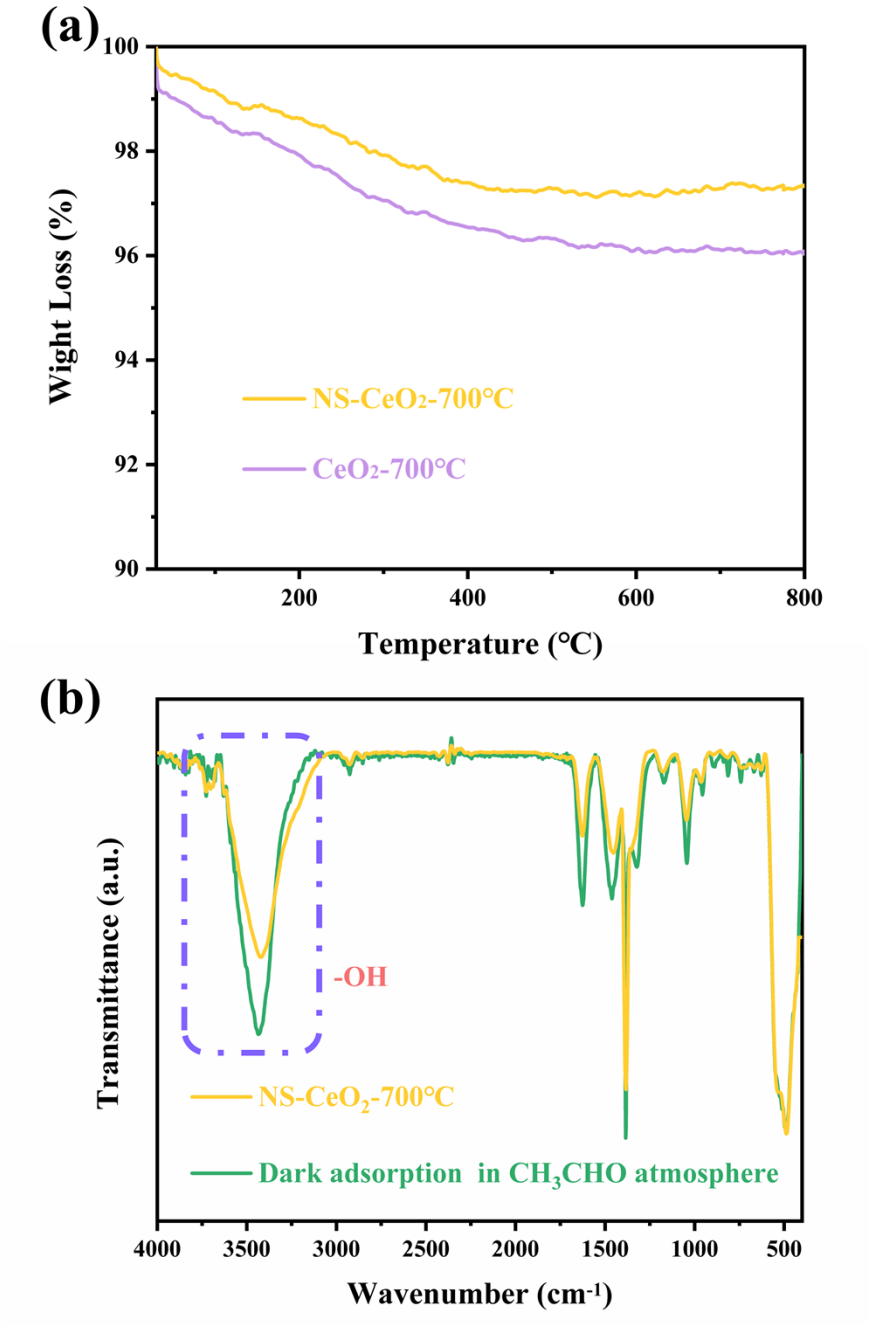

Figure S6. (a) TG curves of NS-CeO_2 and pure CeO_2; and (b) FT-IR spectrum of NS-CeO_2 before and after dark adsorption equilibrium in CH_3CHO atmosphere for 1h.

TG measurement was used to confirm the partial adsorption of water on the surface of the photocatalysts convincingly. In addition, FT-IR spectrum of NS-CeO_2 contained a significant peak at 3450 cm^{-1} and this peak was attributed to the hydroxyl vibration of adsorption of water on the photocatalysts surface. While after dark adsorption equilibrium in CH_3CHO atmosphere for 1h, the stronger characteristic absorption peak of -OH can be clearly observed in NS-CeO_2, indicating a further increase tendency of water content on its surface.

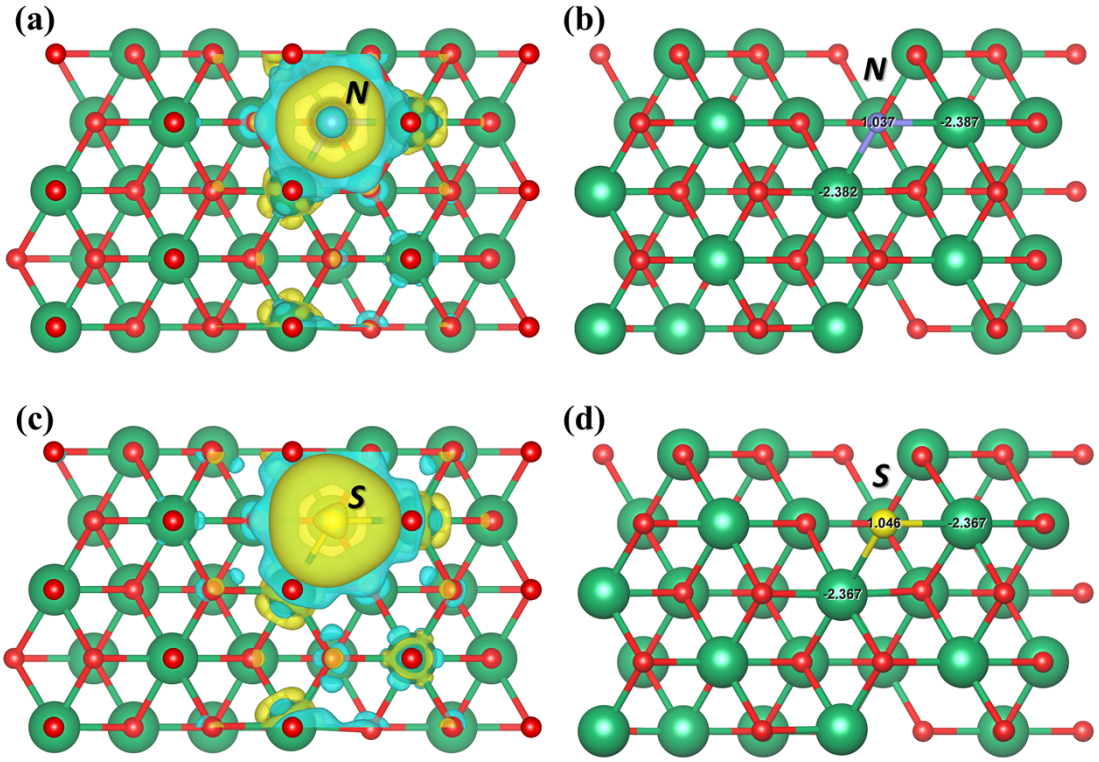

Figure S7. Bader charge diagram and calculated cross view charge density differences of (a, b) N doped-CeO_2 and (c, d) S doped-CeO_2.

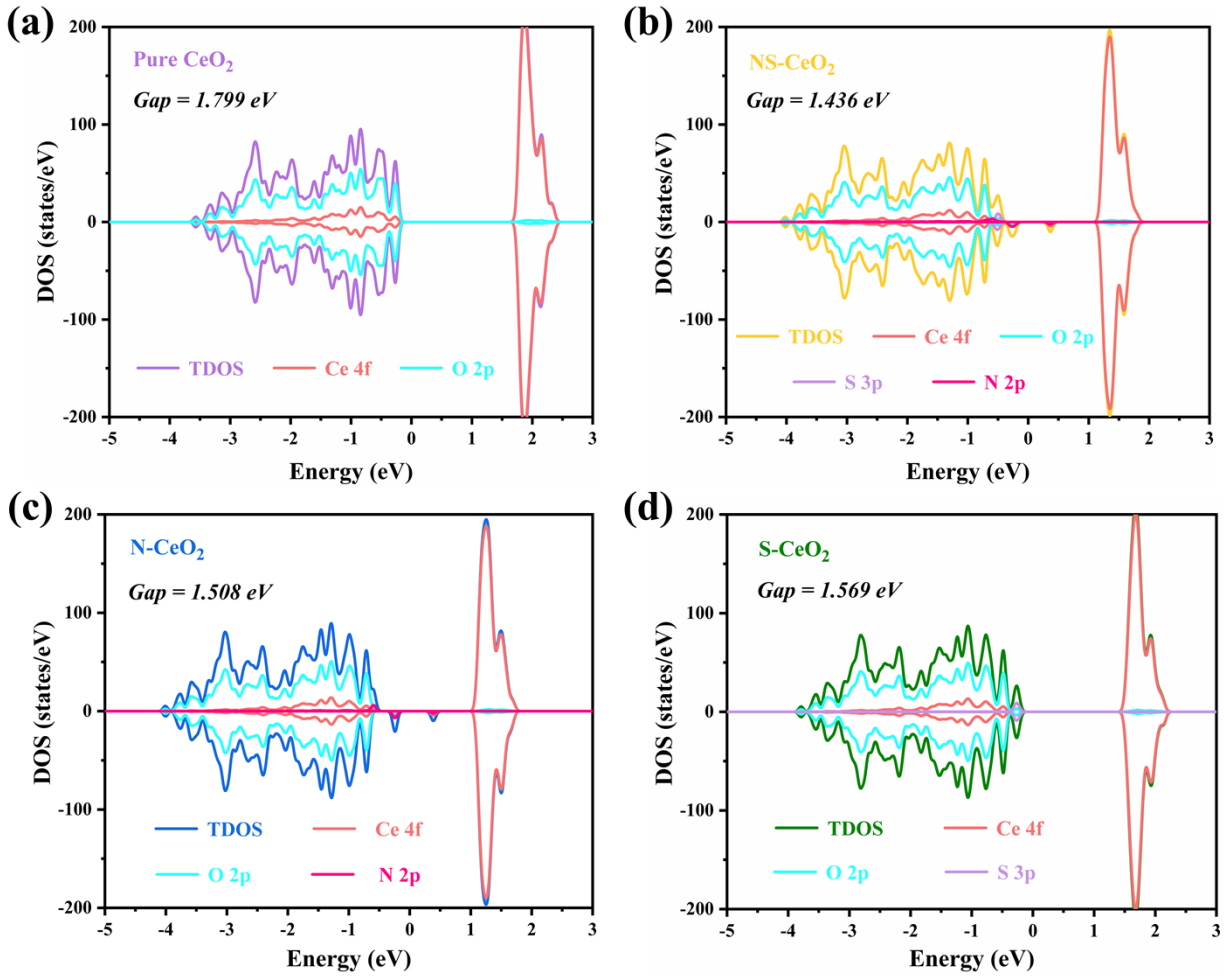

Figure S8. Results for total and partial density of states (DOS) of (a) pure CeO_2, (b) NS-CeO_2, (c) N-CeO_2 and (d) S-CeO_2.s