Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Principles of doping ceria for the solar thermochemical redox splitting of H_2O and CO_2

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Supplementary information

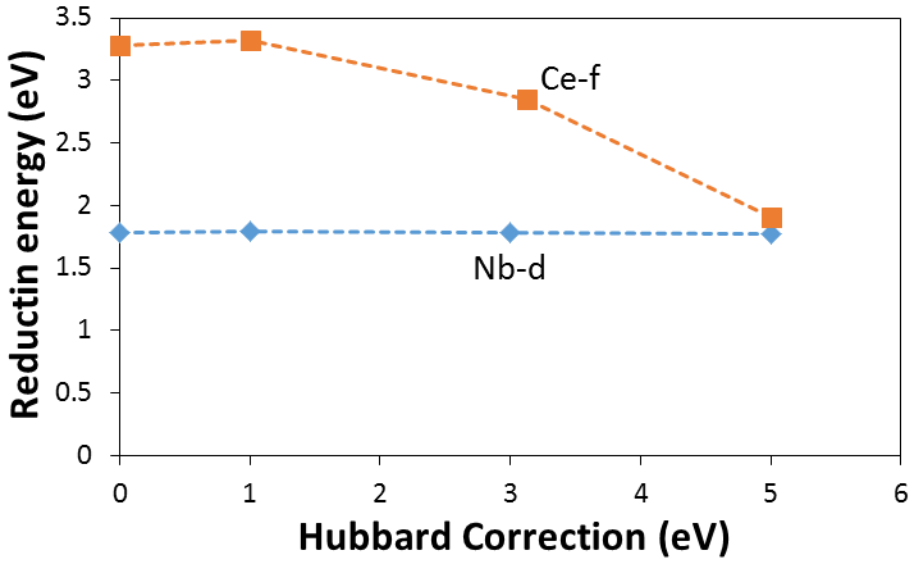


Figure SI 1: Effect of the Hubbard correction values on the O-vacancy formation energy in ceria. Both the effect to various U values on the Nb-d orbitals in Nb-doped ceria (Ce-f orbitals are corrected with U=3.125 eV), and the effect of U on the Ce-f orbital Hubbard in undoped ceria is shown.

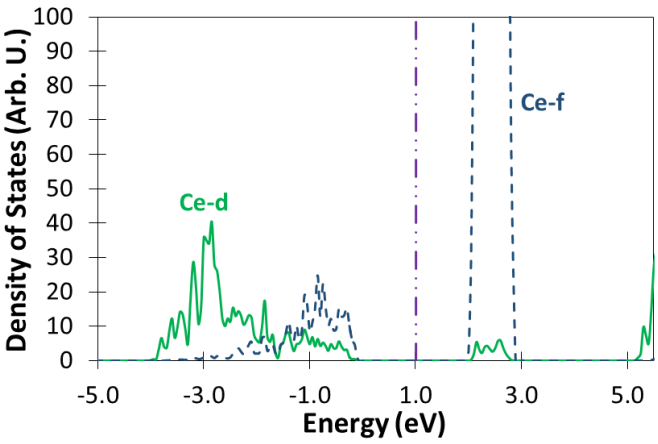
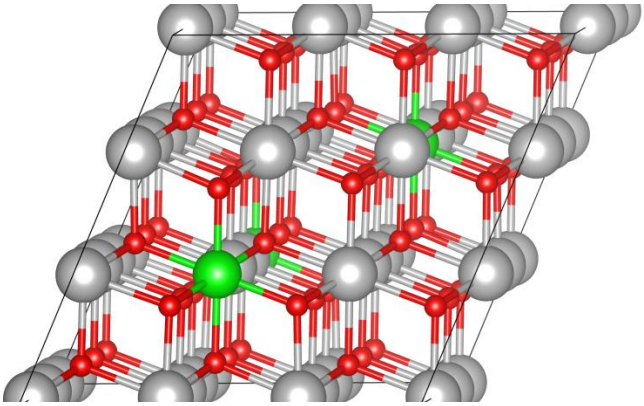


Figure SI 2: Projection of the density of states of undoped oxidized CeO_2 onto Ce d and Ce f orbitals.

a)



b)

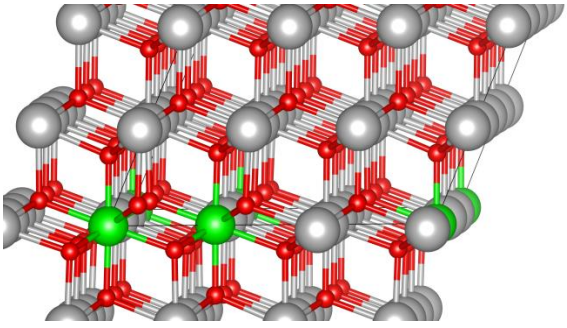


Figure S3. Comparison of the locations of the Zr dopant ions in ceria when two dopants are present. a) shows the “far” configuration and b) shows the “near” configuration. The large gray, medium green and small red spheres represent Ce, Zr, and O ions respectively.

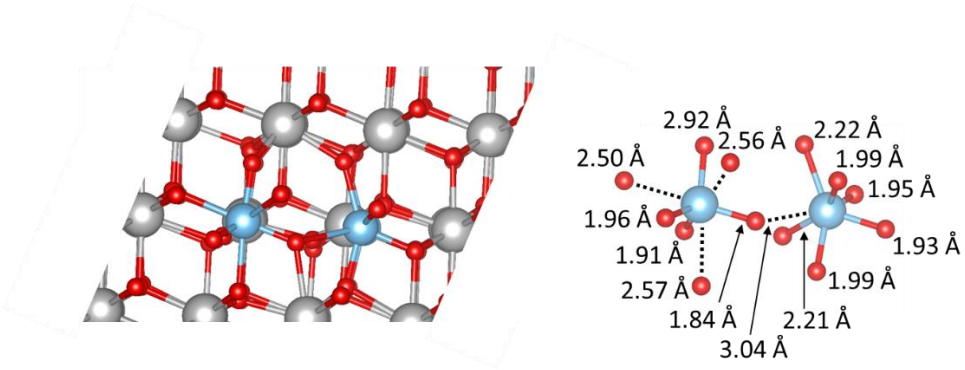


Figure S4. A geometric representation of the reduced Ti-CeO_2 when two Ti cations are paired. More detail and inter atomic distances are provided in the right hand panel. The large gray, medium blue and small red spheres represent Ce, Ti, and O ions respectively.