Electronic supplementary information

Preferential location of zirconium dopants in cerium dioxide nanoparticles and effects of doping on their reducibility: A DFT study

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Table S1. Shift of the O 1s core level energies, ΔE(O 1s) (in eV) of the O centers bound to Zr^{4+} cation in $Ce_{39}ZrO_{80}$ structures with respect to the pristine $Ce_{40}O_{80}$ nanoparticle. Positive values correspond to destabilization of the O 1s core level, i.e. increased basicity of the corresponding oxygen ion.

Structure	ΔE(O 1s)
A	-0.24; -0.23; -0.09; -0.09; -0.02; -0.01
B	-0.17; -0.17; -0.22; -0.23; 0.00; 0.01
C	-0.07; 0.07; 0.07; 0.07; 0.08; 0.10; 0.10
D	-0.09; -0.09; -0.02; -0.02; 0.14; 0.14
E	-0.05; -0.05; -0.04; -0.04
N	0.08; 0.08; 0.08; 0.09; 0.11; 0.12; 0.12; 0.13
L	-0.06; 0.03; 0.03; 0.03; 0.03; 0.09; 0.09; 0.09

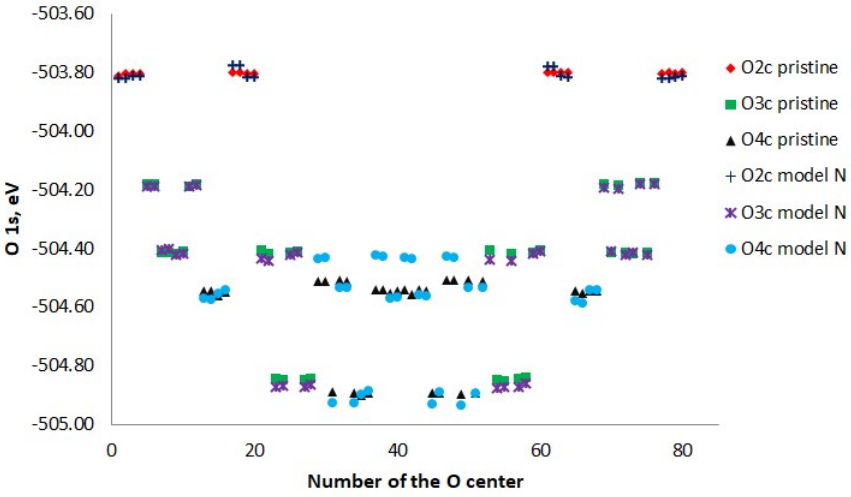
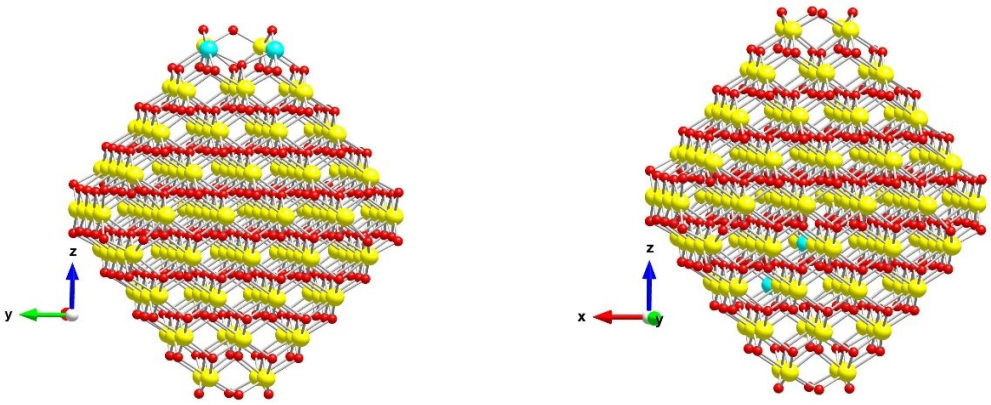
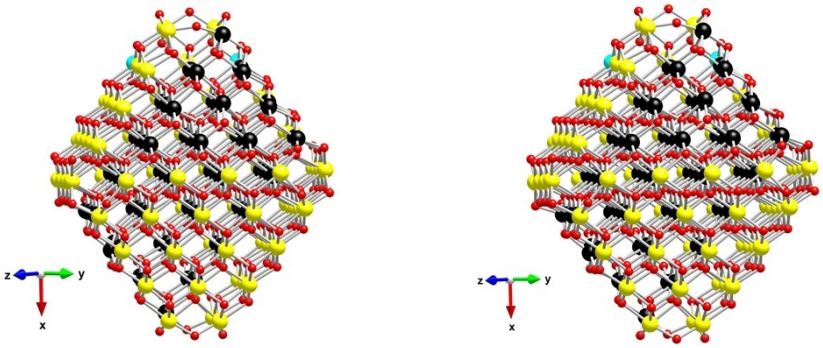


Figure S1. Estimated O 1s core-level energies for the pristine $Ce_{40}O_{80}$ nanoparticle and for the most stable $Ce_{39}ZrO_{80}$ structure – N.

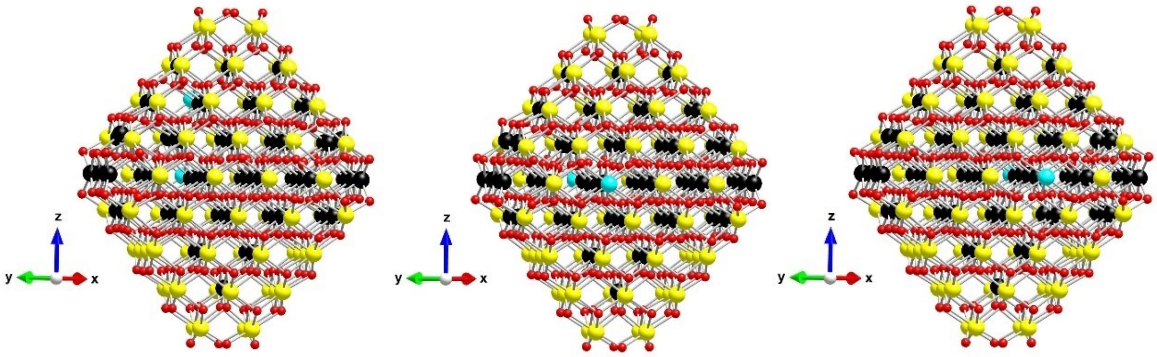


$Ce_{140}O_{280}\_O_{2c}\_d$ $Ce_{140}O_{280}\_O_{4c}\_b$

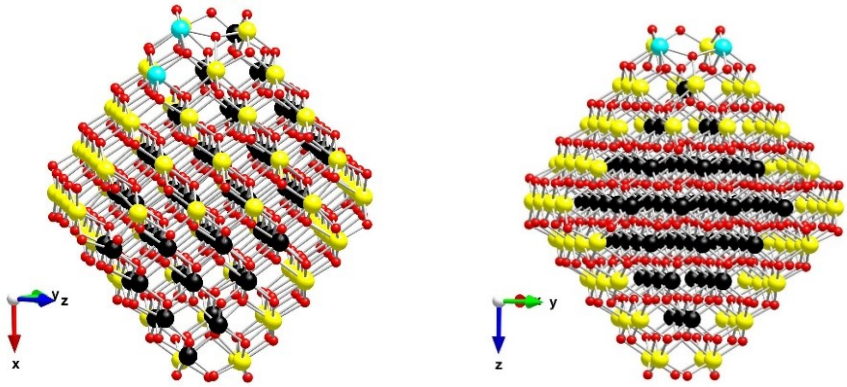
Figure S2. Optimized structures of $Ce_{140}O_{279}$ models. Color coding: Ce^{4+} – yellow, Ce^{3+} – cyan, O – red.



$Ce_{70}Zr_{70}O_{280}\_O_{4c}\_a$ $Ce_{70}Zr_{70}O_{280}\_O_{2c}\_b$



$Ce_{70}Zr_{70}O_{280}\_O_{4c}\_c$ $Ce_{70}Zr_{70}O_{280}\_O_{4c}\_d$ $Ce_{70}Zr_{70}O_{280}\_O_{4c}\_e$



$Ce_{70}Zr_{70}O_{280}\_O_{2c}\_f$ $Ce_{70}Zr_{70}O_{280}\_O_{2c}\_g$

Figure S3. Optimized structures of $Ce_{70}Zr_{70}O_{279}$ models. Colour coding: Ce^{4+} – yellow, Ce^{3+} – cyan, O – red, Zr^{4+} – black.