Electronic Supplementary Information

Structure and stability of reduced and oxidized mononuclear platinum species on nanostructured ceria from density functional modeling

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Content

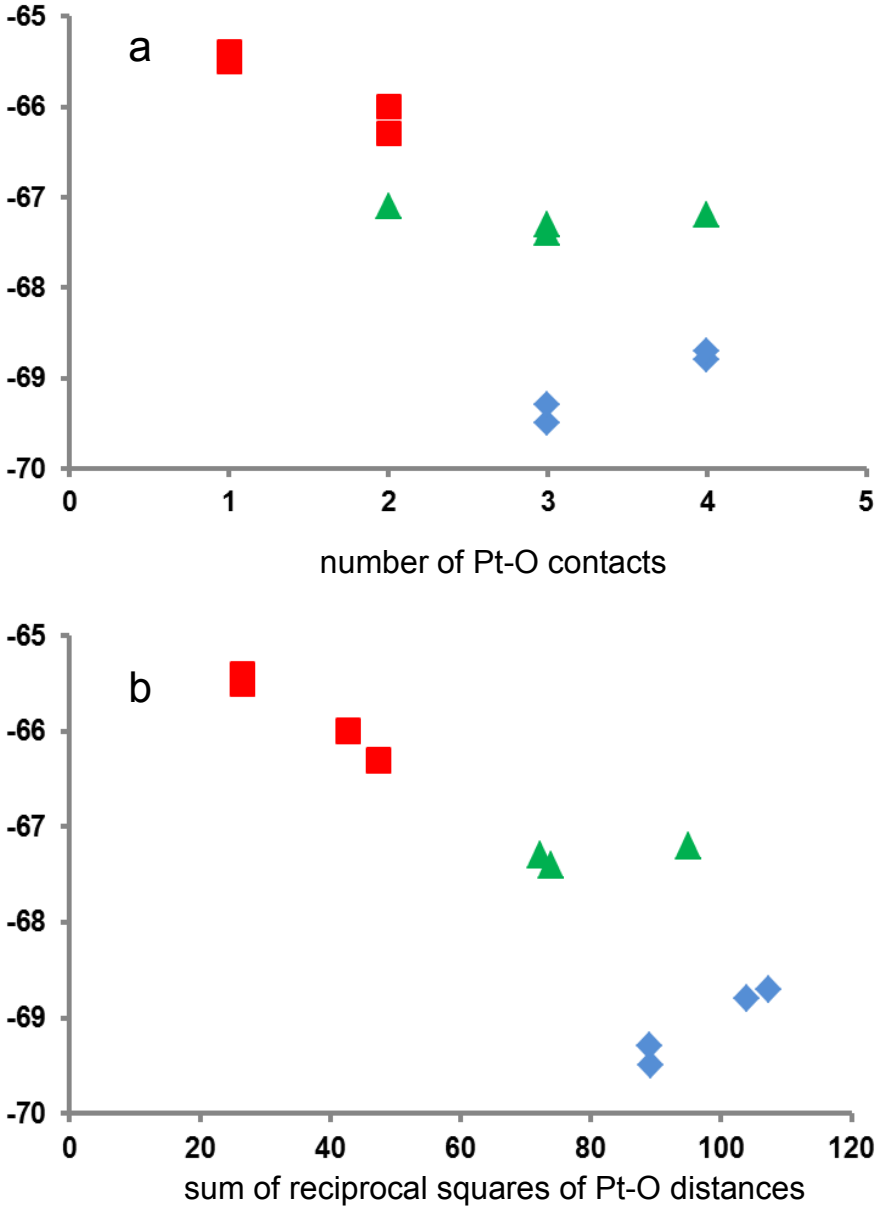
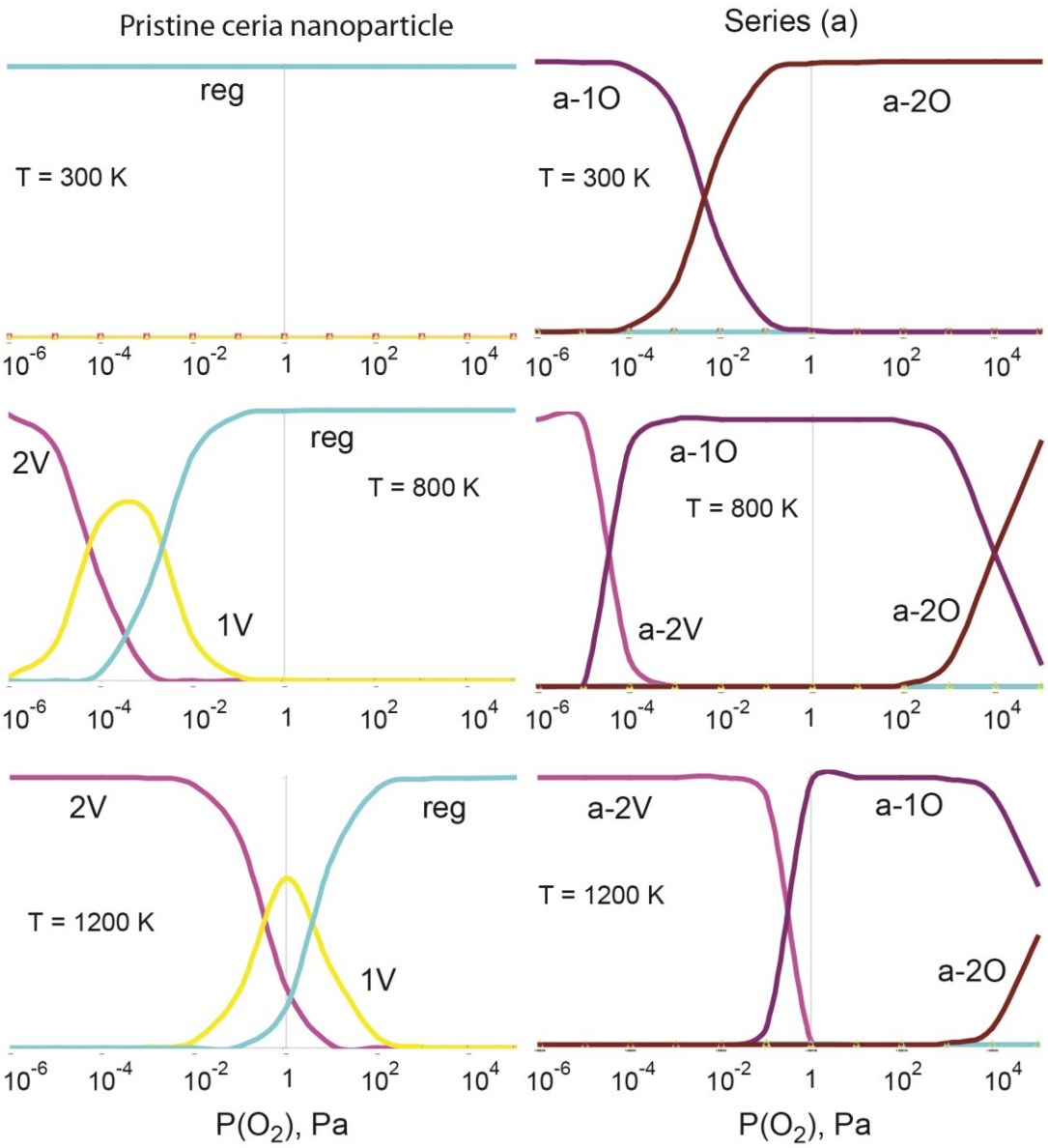
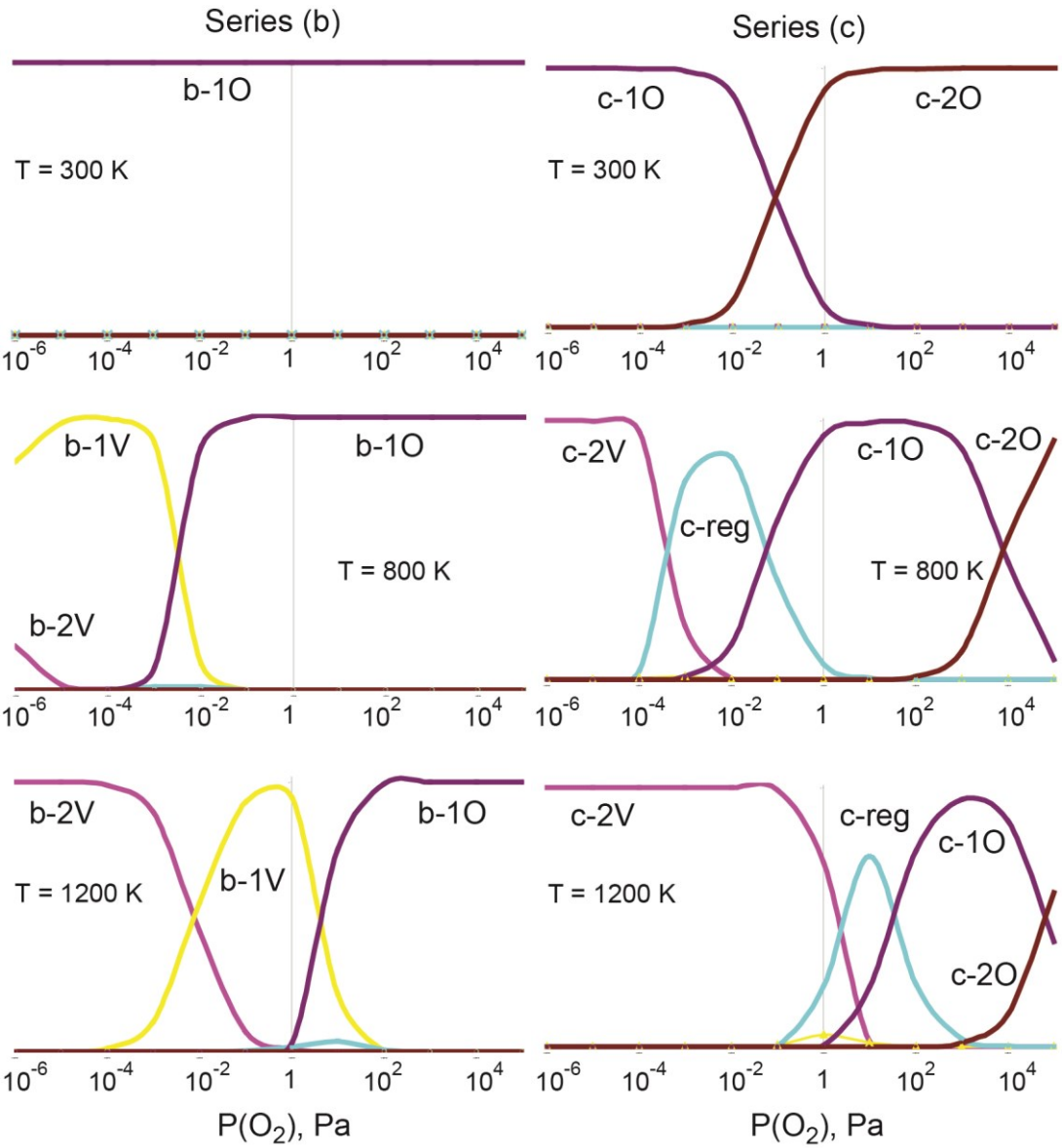


Figure S1

Calculated Pt 4f core level energies of platinum species (with respect to the Fermi level in the system) in eV versus (a) the number of Pt-O contacts or (b) the sum of reciprocal squares of Pt-O distances (in pm^{-2} multiplied by 10^6): species corresponding to Pt^0 (red squares), to Pt^{2+} (green triangles) and Pt^{4+} (blue rhombus).


Pristine ceria nanoparticle
Series (a)
reg
T = 300 K
a-1O
a-2O
T = 300 K
2V
reg
T = 800 K
1V
a-1O
T = 800 K
a-2V
a-2O
2V
reg
T = 1200 K
1V
a-2V
a-1O
T = 1200 K
a-2O
10-6 10-4 10-2 1 102 104
P(O2), Pa


Series (b)
Series (c)
b-1O
T = 300 K
c-1O
c-2O
T = 300 K
b-1V
b-1O
T = 800 K
b-2V
c-2V
c-reg
c-1O
c-2O
T = 800 K
b-2V
b-1O
T = 1200 K
b-1V
c-2V
c-reg
c-1O
T = 1200 K
c-2O
10^-6 10^-4 10^-2 1 10^2 10^4
P(O2), Pa

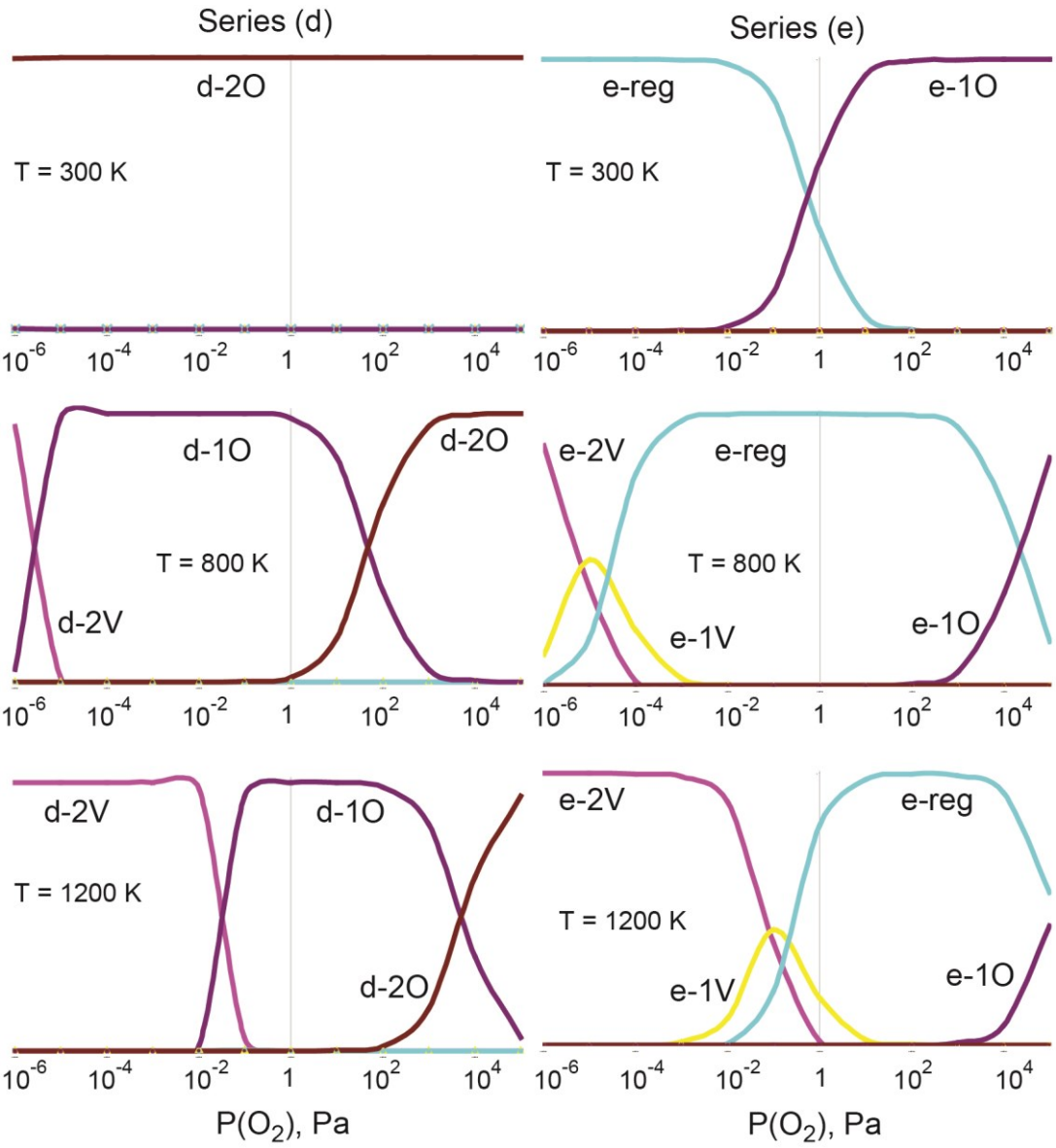


Figure S2
Concentration of various complexes as function of $P(O_2)$ obtained thermodynamic models for the various series $PtO_X/Ce_{21}O_{42-Y}$ (X, Y = 0 ÷ 2): for Y = 0 – 2 and X = 0 and 1 and on the pristine $Ce_{21}O_{42}$ at three different temperatures, 300, 800 and 1200 K. The vertical axis corresponds to the relative concentration of the species ranging from 0 to 100%.