

Electronic and Atomistic Structures of Clean and Reduced

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Citation Report

#	ARTICLE	IF	CITATIONS
4	Effects of Zr doping on stoichiometric and reduced ceria: A first-principles study. Journal of Chemical Physics, 2006, 124, 224704.	1.2	131
5	The Surface Dependence of CO Adsorption on Ceria. Journal of Physical Chemistry B, 2006, 110, 16600-16606.	1.2	172
6	Interaction of Hydrogen with Cerium Oxide Surfaces: a Quantum Mechanical Computational Study. Journal of Physical Chemistry B, 2006, 110, 19380-19385.	1.2	85
7	Hole localization in Al doped silica: A DFT+U description. Journal of Chemical Physics, 2006, 125, 144701.	1.2	113
8	Development of Constraint Algorithm for the Number of Electrons in Molecular Orbitals Consisting Mainly 4f Atomic Orbitals of Rare-Earth Elements and Its Introduction to Tight-Binding Quantum Chemical Molecular Dynamics Method. Japanese Journal of Applied Physics, 2007, 46, 2505-2509.	0.8	8
9	Oxygen vacancy formation energy in Pd-doped ceria: A DFT+U study. Journal of Chemical Physics, 2007, 127, 074704.	1.2	105
10	A First-Principles Analysis for Sulfur Tolerance of CeO ₂ in Solid Oxide Fuel Cells. Journal of Physical Chemistry C, 2007, 111, 11117-11122.	1.5	63
11	Tuning LDA+U for electron localization and structure at oxygen vacancies in ceria. Journal of Chemical Physics, 2007, 127, 244704.	1.2	313
12	Hybrid functionals applied to rare-earth oxides: The example of ceria. Physical Review B, 2007, 75, .	1.1	502
13	Hydrogen Cycle on CeO ₂ (111) Surfaces: Density Functional Theory Calculations. Journal of Physical Chemistry C, 2007, 111, 15337-15341.	1.5	131
14	Modeling of CeO ₂ , Ce ₂ O ₃ , and CeO _{2-x} in the LDA+U formalism. Physical Review B, 2007, 75, .	1.1	333
15	Methanol Adsorption on the Clean CeO ₂ (111) Surface: A Density Functional Theory Study. Journal of Physical Chemistry C, 2007, 111, 10514-10522.	1.5	56
16	Role of surface peroxy and superoxy species in the low-temperature oxygen buffering of ceria: Density functional theory calculations. Physical Review B, 2007, 75, .	1.1	112
17	Evidence of Subsurface Oxygen Vacancy Ordering on Reduced CeO_2 Surfaces: Density Functional Theory Calculations. Journal of Physical Chemistry C, 2007, 111, 15337-15341.	2.9	177
18	Oxygen vacancies in transition metal and rare earth oxides: Current state of understanding and remaining challenges. Surface Science Reports, 2007, 62, 219-270.	3.8	1,102
19	Catalysis by doped oxides: CO oxidation by Au/CeO ₂ . Journal of Catalysis, 2007, 245, 205-214.	3.1	325
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21	A density functional theory study of formaldehyde adsorption on ceria. Surface Science, 2007, 601, 4993-5001.	0.8	44

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23	Facilitated vacancy formation at Zr-doped ceria(111) surfaces. Surface Science, 2008, 602, 1199-1206.	0.8	68
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58	Point defects in CaF_2 and CeO_2 investigated by the periodic electrostatic embedded cluster method. <i>Journal of Chemical Physics</i> , 2009, 130, 174710.	1.2	88
59	Redox properties of gold-substituted zirconia surfaces. <i>Journal of Materials Chemistry</i> , 2009, 19, 710-717.	6.7	12

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87	Formation of Superoxide Anions on Ceria Nanoparticles by Interaction of Molecular Oxygen with Ce ³⁺ Sites. Journal of Physical Chemistry C, 2011, 115, 5817-5822.	1.5	107
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170	Effects of Fe doping on oxygen vacancy formation and CO adsorption and oxidation at the ceria(111) surface. <i>Catalysis Communications</i> , 2015, 63, 35-40.	1.6	28
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172	Role of oxygen vacancies in the surface evolution of H at CeO ₂ (111): a charge modification effect. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 3544-3549.	1.3	73
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