

Abstract Submitted  
for the MAR09 Meeting of  
The American Physical Society

**Density functional calculations of the structure of near-surface oxygen vacancies and electron localization on CeO<sub>2</sub>(111)** M. VERONICA GANDUGLIA-PIROVANO, Humboldt-University Berlin, Unter den Linden 6, 10099 Berlin, Germany, JUAREZ L.F. DA SILVA, National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, CO 80401, USA, JOACHIM SAUER, Humboldt-University Berlin, Unter den Linden 6, 10099 Berlin, Germany — The use of ceria as a key component in catalysts and as an electrolyte for solid oxide fuel cells relies on its notorious capability of storing and releasing oxygen. This property results from the facility of both formation and healing of oxygen vacancies in ceria. Several studies have been reported in the last years for reduced CeO<sub>2</sub>(111), however, one of the most topical issues surrounding oxygen vacancies on CeO<sub>2</sub>(111), namely, the relative stability of surface and subsurface defects, is still under intense debate. Using density functional theory with the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional as well as the DFT+U approach, we find subsurface vacancies with (2×2) periodicity to be energetically more favorable by 0.45 (HSE06), 0.47 (PBE+U), and 0.22 eV (LDA+U). The excess-electrons localize not on Ce ions which are nearest neighbor to the defect as priorly suggested, but instead on those that are next-nearest neighbors. The excess-electron distribution and the preference for subsurface vacancies are explained in terms of defect-induced lattice relaxation effects.

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Date submitted: 11 Dec 2008

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