

Abstract Submitted
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First Principles Study of Energetics, Local Electronic States and Adsorption of H₂O and H₂O₂ on Reduced CeO₂ Surfaces¹ NAN SHAO, University of Nebraska at Omaha, NABIL AL-AQTASH, Hasemite University, Jordan, KHALDOUN TARAWNEH, Princess Sumaya University for Technology, Jordan, CHIN LI CHEUNG, University of Nebraska Lincoln, WAI-NING MEI, RENAT SABIRIANOV, University of Nebraska at Omaha — The importance of ceria (CeO₂) in catalysis originates from its remarkable redox and oxygen storage capability. It undergoes repeatable Ce⁴⁺/Ce³⁺ redox cycles depending on the operation conditions. The great effort has been made to improve ceria reducibility. The reduction of ceria can be controlled by the oxygen vacancies. We study the energetics, local electronic states, and oxygen vacancy formation energies for the (111), (110) and (100) surfaces of stoichiometric and reduced ceria by DFT+U calculations. We find that ceria (111) surface is most stable, while (100) and (110) surfaces have higher formation energies. Both subsurface and surface oxygen vacancies induce the electron localization of reduced CeO₂ on all these three terminations of the surface, leading to the appearance of Ce³⁺ sites. In the case of ceria (111) surface, oxygen vacancy at the surface and subsurface forms Ce³⁺ at next nearest neighbor to the vacancy. This is consistent with the experimental finding that the ratios of these two types of oxygen vacancy are almost same. In the case of ceria (100) and (110) surfaces, Ce³⁺ is formed at the sites nearest to the oxygen vacancy sites. The H₂O and H₂O₂ adsorption and dissociation on three reduced surfaces are also investigated. Ce³⁺ generated by oxygen vacancy can promote the adsorption of H₂O and H₂O₂.

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