Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Interaction of small polarons and oxygen vacancies in CeO2 LU SUN, Univ of Delaware, LIGEN WANG, General Research Institute for Nonferrous Metals, ANDERSON JANOTTI, Univ of Delaware — The properties that make cerium oxide (CeO2) a promising material for solid oxide fuel and electrochemical cells are closely related to the easy of oxygen vacancy formation and Ce4+ $\leftrightarrow$Ce3+ conversion, i.e., small polaron formation. The effects of oxygen vacancy on the structure and electronic properties of CeO2 have been extensively studied from both experiment and theory, yet vacancy formation energy and parameters of the polaron-vacancy interaction vary over a wide range. Using first-principles calculations based on hybrid functional, we investigate the formation and migration of small polarons (Ce3+) and their interaction with oxygen vacancies in CeO2, treating the small polaron and vacancy as independent entities. We compute the electron self-trapping energy (i.e., energy gain when forming a small polaron), the small-polaron migration barrier, vacancy formation and migration energies, and vacancy-polaron binding energies. We find that small polarons weakly bind to oxygen vacancies, providing a relatively small contribution to the activation energy barrier for the observed hopping electronic conductivity. The results are compared to previous calculations and discussed in the light of available experimental data.

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Date submitted: 11 Nov 2016 Electronic form version 1.4