

Abstract Submitted
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Density functional theory study of defect energies and space charge distribution at a solid-oxide electrolyte surface CHU HAN, ANGELO BONGIORNO, Georgia Institute of Technology — Yttrium-doped barium zirconate (BZY) is a proton conducting electrolyte forming a class of novel materials for new generation of solid oxide fuel cells, for hydrogen separation and purification, and for electrolysis of water. Here we use density functional theory calculations to compute the energy of protons and oxygen vacancies at the surface and in the bulk of lightly Y-doped BZY materials. We found that protons are energetically more stable at the surface termination than in the bulk of BZY by about 1 eV. In contrast, doubly-positively charged oxygen vacancies are found to form iso-energetic defects at both the terminal surface layer and in the bulk of BZY, while in the sub-surface region the defect energy raises by about 1 eV with respect to the value in the bulk. The energetic behavior of protons and oxygen vacancies in the near surface region of BZY is attributed to the competition of strain and electrostatic effects. Lattice model representations of BZY surfaces are then used in combination with Monte Carlo simulations to solve the Poisson-Boltzmann equation and investigate the implication of the results above on the structure of the space charge region at the surface of BZY materials.

Chu Han
Georgia Institute of Technology

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