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Impact of Applied Electric Bias on Oxygen Reactivity and Oxide Diffusion at Lanthanum Strontium Manganite Electrode Surfaces

Lanthanum Strontium Manganite (LSM) is a widely used cathode material in solid oxide fuel cells (SOFCs) due to its stability and catalytic activity in oxygen redox reaction (ORR) [1, 2]. Although its surface properties have been extensively studied [3], the effects of electric polarization on chemical reactivity and oxide diffusion remain largely unexplored. In this study, we employ state-of-the-art density functional theory (DFT) calculations with an applied electric field [4] to investigate the structural, electronic, and catalytic properties of the pristine and defective LSM (001) surface, focusing on oxygen migration and vacancy dynamics. We first characterize the surface geometry and electronic structure, assessing how surface reconstitution and oxygen vacancy formation energies influence catalytic activity. To simulate realistic SOFC conditions, we apply an external electric field during both vacancy formation energy calculations and climbing-image nudged elastic band (CI-NEB) simulations to model oxide ion migration. Additionally, we examine the ORR on both pristine and defective LSM surfaces under applied potentials, elucidating the role of vacancies in modulating catalytic activity. Our findings reveal how polarization and surface-specific effects influence oxygen transport and ORR kinetics, providing a more comprehensive picture of LSM's catalytic behavior. By integrating advanced computational techniques with an electrochemical perspective, this work offers valuable insights on the possible modulation of LSM electrocatalytic properties via electric bias, and contributes to the rational design of more efficient cathode materials for application in SOFCs.

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