ISBN:
978-1-917892-14-8

4th International Conference on Chemistry & Chemical Engineering

July 21-22, 2025 | Paris, France

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Empirical Potential Influence on Proton Transfer and Trapping in Scandium-Doped Barium Zirconate with Oxygen Vacancies

Abstract: Scandium-doped barium zirconate ($BaZrO_3$) is a promising material for hydrogen fuel cells due to its high proton conductivity, warranting further investigation into the influence of oxygen vacancies on the proton conduction landscape. This study employs empirical interatomic potentials to identify geometric and energetic factors governing local proton mobility and long-range diffusion through analysis of intraoctahedral transfers, transition energy barriers, and site energetics. Sites within 2–4 Å of an oxygen vacancy were prone to proton trapping, driven by increased octahedral tilting and the formation of multidirectional bonding environments. Transition state analyses revealed distinct energy profiles across single-, bi-, and unidirectional proton interactions, with unidirectional pairs exhibiting inverted barriers that hinder net conduction. A systematic comparison demonstrated that, relative to Buckingham potential, the Morse (Gale, Islam) potentials introduce larger energy fluctuations and more pronounced interaction cutoff dependence, especially for O-H interactions. Rotational and translational barriers diverge in their cutoff preferences, suggesting trade-offs in empirical parameter selection. Centrality and Kinetic Monte Carlo simulations further confirm that steeper Morse parameters suppress diffusive motion. These findings underscore the importance of potential tuning and local structural descriptors in capturing the complex conduction behavior of proton-conducting perovskites.

Keywords: proton conduction, fuel cells, perovskites, computational

Biography: As an undergraduate chemistry student at Mount Holyoke College, Carlyn Danese studies polymer thin film crosslinking under Dr. Wei Chen and perovskite proton conduction under Dr. Maria Gomez. Carlyn is also serving as a DAAD RISE Fellow in Germany this summer, investigating surface modifications of porous carbon materials at the Helmholtz Institute for Polymers in Energy Applications.