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ABSTRACT:

Impact of Defect Interactions on Thermodynamics and Kinetics in Solid State Ionics

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Defect–defect interactions are a fundamental determinant of both thermodynamic stability and kinetic transport in solid-state ionics. These interactions significantly influence defect formation energetics and charge carrier mobility, particularly in oxides with high, dopant-induced defect concentrations. Understanding these phenomena is critical for the advancement of technologies such as gas sensors, electrolyzers, and solid oxide fuel cells. In this field, computational methods offer unique, detailed insights into the mechanisms of defect interactions and their subsequent impact on macroscopic properties.

This presentation provides a comprehensive overview of our recent computational investigations into defect chemistry and ion transport across representative oxide systems, namely pure and doped ceria as well as doped barium zirconate.[1]

Our research utilizes a multiscale approach, integrating Density Functional Theory (DFT) with Metropolis Monte Carlo (MMC) and Kinetic Monte Carlo (KMC) simulations. This methodology bridges the gap between atomistic defect energetics and mesoscale transport behavior. By establishing this link, we provide mechanistic insights into how defect association, clustering, and specific migration pathways collectively dictate macroscopic ionic conductivity.

[1] S. Neitzel-Grieshammer, M. Martin, Solid State Ionics, 438, 117152 (2026).