Contribution ID : **179** Type : **Poster Presentation**

EuCompChem2025 – Sara Balocco – Oral

Solid oxide fuel cells (SOFCs) and their reversible counterparts, solid oxide electrolyzer cells (SOECs), offer efficient routes for clean energy conversion water splitting and hydrogen storage [1]. However, efficient transport of oxygen ions and electrons in state-of-the-art solid-state electrolytes and electrodes typically requires high temperatures, which limit device durability and slow start-up times. Lowering the operating temperature necessitates advanced electrode materials, particularly mixed ionic-electronic conductors (MIECs) [2]. Among these, perovskite oxides have emerged as promising electrodes for both the oxygen evolution and reduction reactions (OER/ORR), though the efficiency of the two opposite reactions being usually largely different. Sr2Fe1.5Mo0.5O6-δ (SFMO) has attracted attention as a potentially bifunctional system due to its high electronic conductivity, redox-active B-site cations (Fe/Mo), and capacity to accommodate oxygen vacancies. Following previous works [3, 4], in this study, we investigate the impact of cationic substitution on oxygen vacancy formation and migration in SFMO via first-principles calculations, targeting improved oxygen ion transport. Two Fe:Mo ratios (1:1 and Fe-rich 3:1) are considered to assess the effect of B-site composition, while partial substitution of A-site cation (Sr) with smaller (Ca) and larger (Ba) cations at two Sr:Ca:Ba ratio (6:1:1 and 4:2:2) allowed us to probe the role of lattice strain. Structural, electronic and energetic properties are investigated using Density Functional Theory (DFT+U), revealing trends relevant to the optimization of SFMO as a bifunctional electrode material for low-temperature solid oxide technologies.

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