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**Atomistic Modeling of Cation Diffusion in Transition Metal Perovskites  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_{3\pm\delta}$  for Solid Oxide Fuel Cell Cathodes Applications** YUEH-LIN LEE, YUHUA DUAN, Natl Energy Technology Lab, DANE MORGAN, Department of Materials Science and Engineering, University of Wisconsin, DAN SORESCU, HARRY ABERNATHY, Natl Energy Technology Lab — Cation diffusion in  $\text{La}_{1-x}\text{Sr}_x\text{MnO}_{3\pm\delta}$  (LSM) and in related perovskite materials play an important role in controlling long term performance and stability of solid oxide fuel cell (SOFCs) cathodes. Due to sluggish rates of cation diffusion and complex coupling between defect chemistry and cation diffusion pathways, currently there is still lack of quantitative theoretical model predictions on cation diffusivity vs. T and  $P(\text{O}_2)$  to describe experimental cation tracer diffusivities. In this work, based on *ab initio* modeling of LSM defect chemistry and migration barriers of the possible cation diffusion pathways, we assess the rates of A-site and B-site cation diffusion in a wide range of T and  $P(\text{O}_2)$  at  $x=0.0$  and  $0.2$  for SOFC applications. We demonstrate the active cation diffusion pathways in LSM involve cation defect clusters as cation transport carriers, where reduction in the cation migration barriers, which are governed by the steric effect associated with the metal-oxygen cage in the perovskite lattice, is much greater than the penalty of repulsive interaction in the A-site and B-site cation vacancy clusters, leading to higher cation diffusion rates as compared to those of single cation vacancy hopping mechanisms. The predicted Mn and La/Sr cation self-diffusion coefficients of LSM at  $x=0.0$  and  $0.2$  along with their  $1/T$  and  $P(\text{O}_2)$  dependences, are in good agreement with the experimental tracer diffusion coefficients.

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