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Designing brownmillerite $SrCoO_{2.5}$(BM-SCO) as a cathode material – a first principles study of oxygen diffusion process in BM-SCO[1]

CHANDRIMA MITRA, TRICIA MEYER, HO NYUNG LEE, FERNANDO REBOREDO, Oak Ridge National Laboratory — The discovery and design of new materials for next generation energy devices are crucial steps towards addressing various energy-related issues. $ABO_{3-\delta}$ type perovskite oxides have emerged as promising candidates for cathode/electrolyte materials in solid oxide fuel cells (SOFC's). In this work, we investigate oxygen diffusion in brownmillerite oxide $SrCoO_{2.5}$ (BM-SCO), employing a first principles approach. Our calculations indicate highly anisotropic diffusion pathways, which result from its anisotropic crystal structure. The one-dimensional vacancy channels are found to provide the easiest route for diffusion. We consider transport via additional oxygen vacancies as well and find the lowest migration barrier to occur within the two dimensional plane of the octahedral coordination of Co. We further find that an important parameter that could control oxygen stoichiometry in BM-SCO, is strain. This has important implications on the migration barrier of oxygen within BM-SCO and hence on the diffusion coefficient.

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