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Anisotropic O vacancy formation and diffusion in LaMnO3 OMOTAYO SALAWU, LIYONG GAN, UDO SCHWINGENSCHLOGL, King Abdullah Univ — Anisotropy effects in solid oxide fuel cells are typically not considered because of the high operating temperatures. Focusing on the prototypical perovskite $LaMnO_3$, we apply first-principles calculations to demonstrate that this approximation is no longer valid when the operating temperature is reduced and discuss the consequences for the material properties. In addition, we show that strain and Sr doping can be used to further increase the anisotropy. Tensile strain promotes both the O formation and diffusion in pristine and Sr doped $LaMnO_3$, while Sr doping enhances the O vacancy formation but not the diffusion barrier. Both in $LaMnO_3$ and $La_{0.75}Sr_{0.25}MnO_3$ the O diffusion is found to be favorable in the [011] and [$0\bar{1}1$] directions.

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