Supplementary Information:

To systematically analyze the effect of temperature on oxygen anion diffusion, MD simulations were performed on $Sr_{0.95}TiO_{3-\delta}$ structures co-doped with Ca^{2+} and La^{3+} within a temperature range of 973K to 1373K. Two specific A-site deficient compositions, $La_{0.05}Sr_{0.85}Ca_{0.05}TiO_{3-\delta}$ (Ca5La5) and $La_{0.10}Sr_{0.60}Ca_{0.25}TiO_{3-\delta}$ (Ca25La10), were chosen for this investigation, as their oxygen anion diffusivity coefficients were found to be comparable to those of the undoped 5% A-site deficient $Sr_{0.95}TiO_{3-\delta}$. The MSD plots corresponding to different temperatures, illustrated in Figures S1 (a) and S2 (a), provide insights into the thermal activation of oxygen ion migration in both co-doped compositions. The calculated oxygen diffusivity coefficients, summarized in Table S1, exhibit a systematic increase with temperature, following an expected thermally activated transport mechanism. This trend suggests that oxygen vacancy migration in the perovskite lattice is enhanced at elevated temperatures due to increased thermal energy overcoming migration barriers. Additionally, the Arrhenius plots, depicted in Figures S1 (b) and S2 (b), were utilized to determine the activation energy (E_a) for oxygen anion diffusion. The linear fit of the diffusivity data in the Arrhenius plots confirms that the oxygen ion conduction mechanism in these co-doped compositions adheres to exponential temperature dependence, as predicted by classical diffusion theory.

Composition	973 K	1073 K	1173 K	1273 K	1373 K
$La_{0.05}Sr_{0.85}Ca_{0.05}TiO_{3-\delta}$ (Ca5La5)	$5.43x10^{-13}$	$6.44x10^{-13}$	$2.11x10^{-12}$	$3.15x10^{-12}$	$7.91x10^{-12}$
$La_{0.10}Sr_{0.60}Ca_{0.25}TiO_{3-\delta}$ (Ca25La10)	$5.37x10^{-13}$	$1.01x10^{-12}$	$2.62x10^{-12}$	$3.58x10^{-12}$	$7.47x10^{-12}$

Table S1. Oxygen anion diffusivity (in m^2/s) at different temperatures for two different compositions of and Ca^{2+} and La^{3+} co-doped $Sr_{0.95}TiO_{3-\delta}$.

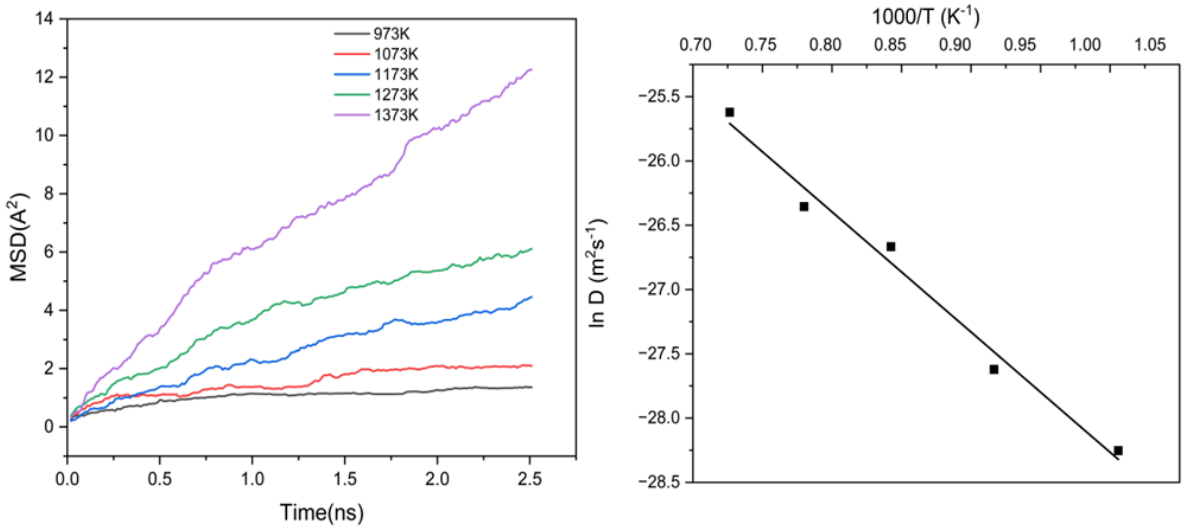

Figure S1 (a) MSD vs time and (b) Arrhenius plot for Ca5La5 (E_a=0.75 eV)

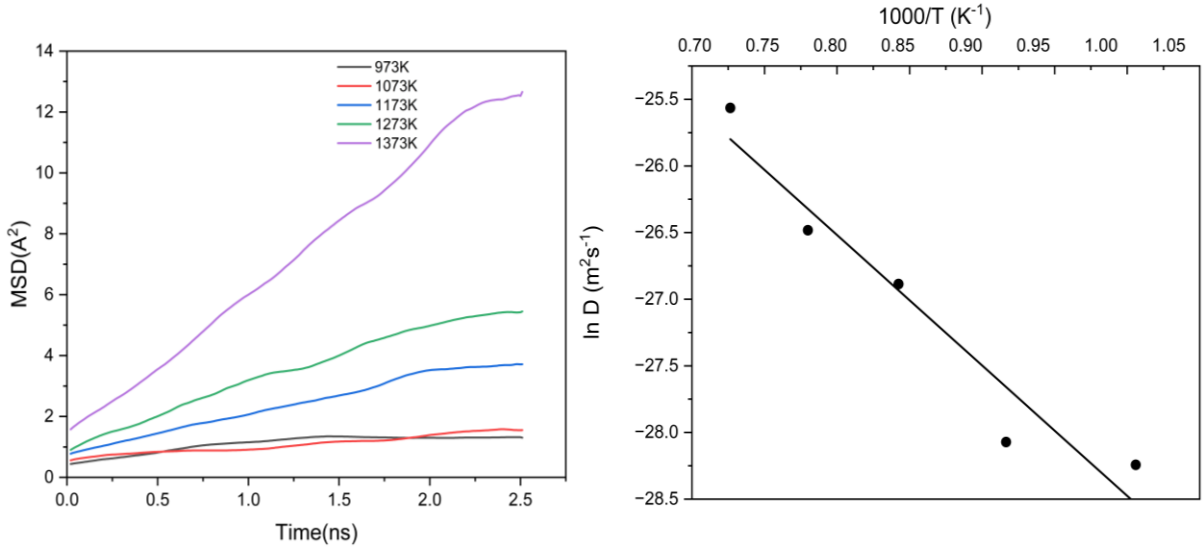

Figure S2 (a) MSD vs time and (b) Arrhenius plot for Ca25La10 (E_a=0.79 eV)