Supplementary Information (SI) for Physical Chemistry Chemical Physics.

# -Supporting Information-

## Molecular Dynamics Studies of Oxide Ion Transport in $Sr$-doped $LaFeO_3$: Role of Cationic Environments and Cooperativity

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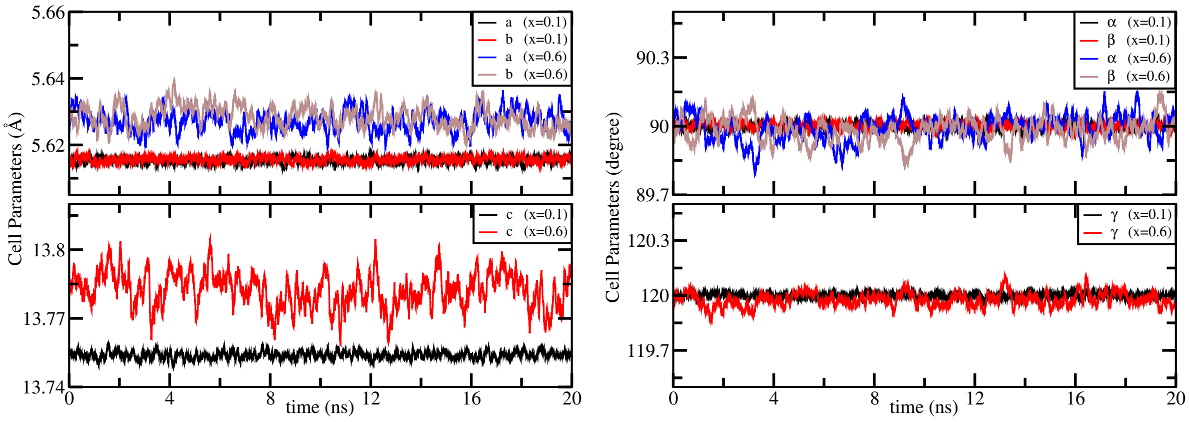

Figure S1: The time evolution of the Rhombohedral unit cell parameters of $La_{1-x}Sr_xFeO_{3-x/2}$ during the 20 $ns$ of NPT-MD simulation at 1200 K, is shown for the end compositions $x$=0.1 and 0.6. The stable evolution of the cell edges and cell angles, except for their fluctuations around the mean, demonstrates the structural stability of the system.

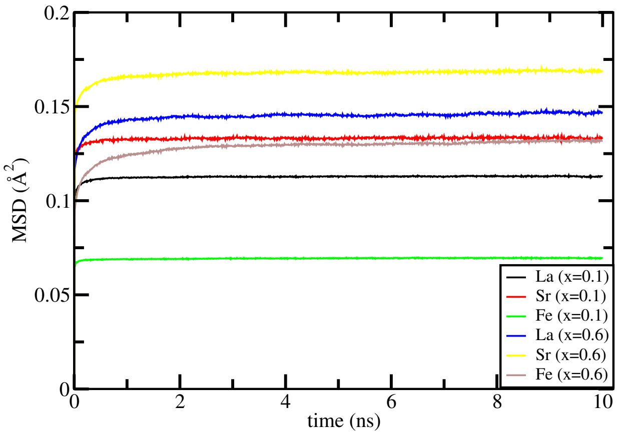

Figure S2: The mean squared displacements (MSDs) of the framework cations ($La$, $Sr$, and $Fe$) at 1200 K, for $x$=0.1 and 0.6, suggest that they are immobile in the matrix, furnishing further evidence for the structural stability of the simulated system at 1200 K.

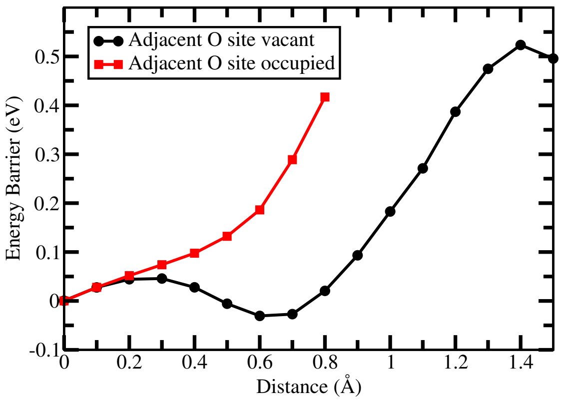

Figure S3: *Left*: Energy profile of oxygen ion when the adjacent site is vacant (black), and when the adjacent sites are occupied (red). As seen, the intermediate minima in the profile vanishes when the adjacent sites (red) are occupied. In this scenario, the ion doesn't make a successful hop, leading to the truncation of the profile by about 0.8 Å from the original site.

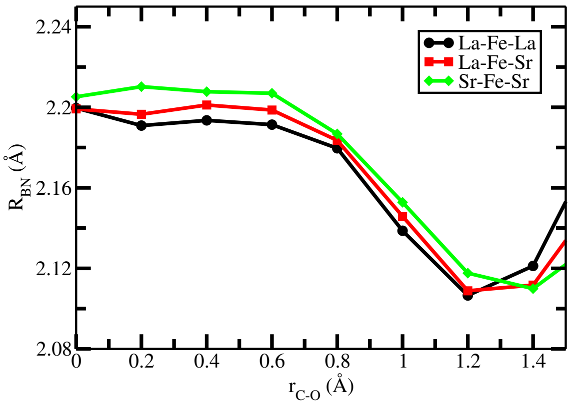

Figure S4: The MD averaged circumradius of bottleneck, $R_{BN}$, as a function of the distance of the approaching oxide ion, $r_{C-O}$, for the three types of bottlenecks, $La - Fe - La$, $La - Fe - Sr$ and $Sr - Fe - Sr$, in $La_{1-x}Sr_xFeO_{3-x/2}$, where $x$=0.6, at 1200 K. As seen, the sizes of these bottlenecks are quite similar.