*Supplementary Information*

# Computational and Experimental Analysis of $Ba_{0.95}La_{0.05}FeO_{3-\delta}$ as a Cathode Material for Solid Oxide Fuel Cells

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This supplementary information contains 3 sections. Section 1 lists the potential parameters used in the manuscripts as well as the reference for each potential parameter. Section 2 contains the information of the temperature fluctuations that are observed in our MD simulation. The last section is about the MD method we used to compute the Poisson's ratio.

**1. The potential parameters**

The Buckingham potential is used in the paper, which adopts the following analytic form.

$$\Phi_{\alpha\beta} = \frac{Z_\alpha Z_\beta e^2}{4\pi\epsilon r_{\alpha\beta}} + A_{\alpha\beta}\exp(-\frac{r_{\alpha\beta}}{\rho_{\alpha\beta}}) - \frac{C_{\alpha\beta}}{r_{\alpha\beta}^6} \quad (1)$$

The parameters for each ionic pair are obtained from the references, as detailed in **Table S1.**

**Table S1**. The potential parameters for the Buckingham pairwise potential.

| Ion pairs | $A_{\alpha\beta}$ / eV | $\rho_{\alpha\beta}$ / nm | $C_{\alpha\beta}$ / eVÅ$^6$ | Ref. |
|---|---|---|---|---|
| $O^{2-}$---$O^{2-}$ | 22764.3 | 0.1490 | 43.00 | [1] |
| $Ba^{2+}$---$O^{2-}$ | 1214.4 | 0.3522 | 0 | [1] |
| $Fe^{3+}$---$O^{2-}$ | 1156.36 | 0.3299 | 0 | [1] |
| $La^{3+}$---$O^{2-}$ | 1439.7 | 0.3651 | 0 | [2] |
| | 2051.32 | 0.3459 | 15.51 | [3] |
| | 1545.21 | 0.3590 | 0 | [4] |
| | 1439.7 | 0.3661 | 0 | [5] |
| | 2088.79 | 0.3460 | 23.25 | [6] |
| $Y^{3+}$---$O^{2-}$ | 1766.40 | 0.33849 | 19.43 | [7] |
| $Gd^{3+}$---$O^{2-}$ | 1885.75 | 0.3399 | 20.34 | [7] |
| $Sm^{3+}$---$O^{2-}$ | 1944.44 | 0.3414 | 21.49 | [7] |

**2. Fluctuations of molecular dynamics simulation using NPT ensemble**

The fluctuations of molecular dynamics simulation using NPT ensemble are quantified by monitoring the temperature. Figure S1 shows the temperature fluctuations at different target temperatures. For the simulation cases with T = 1173, 1273, 1373, 1473 and 1573 K, the average temperatures, denoted by μ, matched well with the target temperatures, while the fluctuations, reflected by the standard deviation σ, are less than 5% of the target temperature, indicating that well-converged

simulations are obtained.

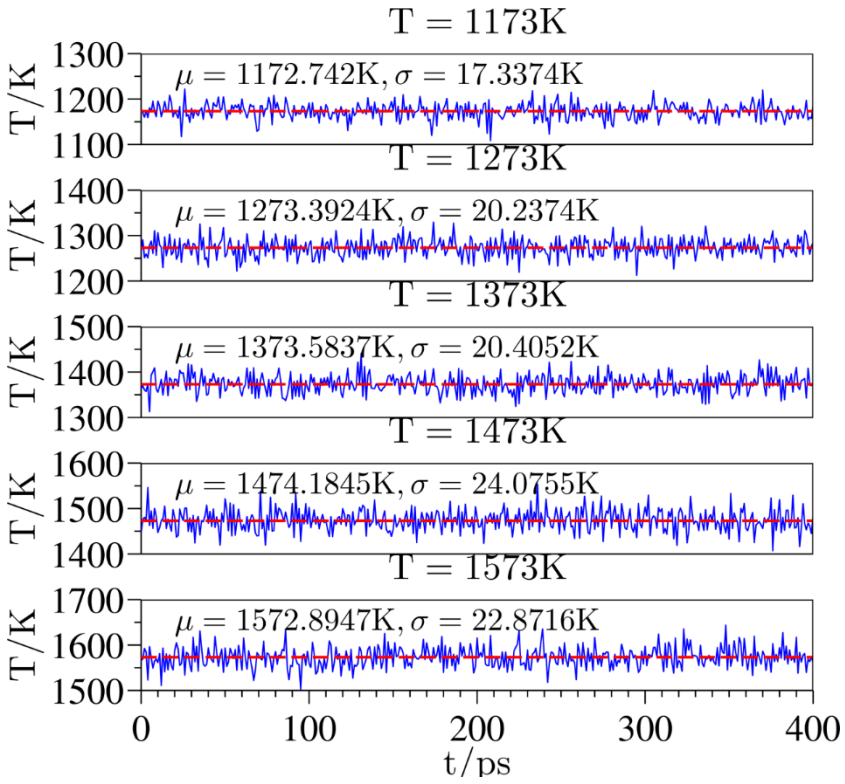


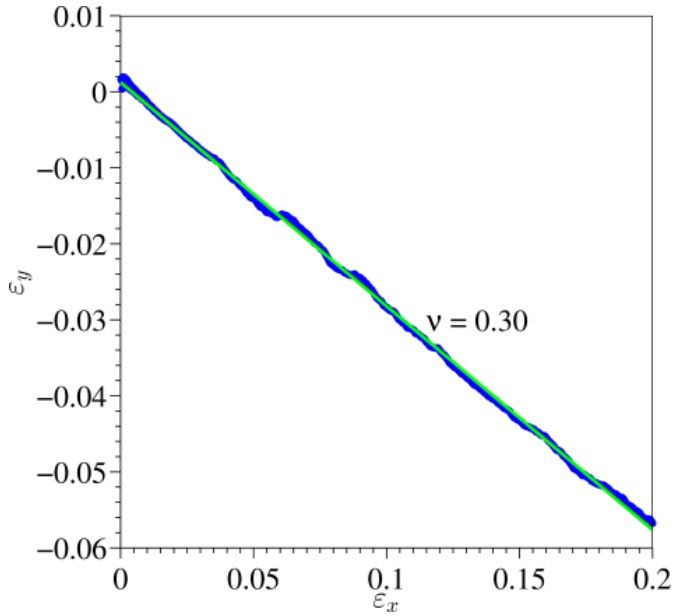

**Figure S1.** Temperature fluctuations of molecular dynamics simulation.

**3. Calculate the Poisson's ratio**

The calculation is implemented in LAMMPS. Besides the conditions mentioned in the main text, the system is modeled by applying a constant uniaxial tensile strain, with a strain rate of $2 \times 10^{-2}/\mathrm{ps}$, for 10 ps (10000 steps). The method is similar to that described in the LAMMPS tutorial page [8]. Once the system is deformed, the engineering strain of each dimension can be measured. The Poisson's ratio is calculated by the equation:

$$\varepsilon_y = -\nu\varepsilon_x \tag{2}$$

where $\varepsilon_x$ is the strain of the loading direction and $\varepsilon_y$ is the transverse direction.




**References**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