Supporting Information

Resolving the Temperature and Composition Dependence of Ion Conductivity for Yttria-Stabilized Zirconia from Machine Learning Simulation

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Table S1. Peak conductivity of YSZ from literatures using MD simulations with empirical potentials

References	Peak conductivity	Model (atoms)	Empirical potentials	mol%Y_2O_3
1995, X. Li,et al[1]	5YSZ for PII at 1500K; 11YSZ for PII at 900K; 8 YSZ for PIII at 900K; 15YSZ for PIII at 1500K	<324	BMH (PI-Butler[2]; PII-Cormack,Catlow[3]; PIII-Dwivedi,Cormack[4])	4.85, 8.00, 11.34, 14.89, 20.00
1999, Yamamura et al[5]	8YSZ at 1273 K	<324	BMH (Brinkman et al)[6]	5.9, 8.0, 10.2, 12.5
2000,Sawaguchi and Ogawa[7]	~11YSZ above1500K;	<1500	BMH(Dwivedi, Cormack[4])	0~29.9
2003,Kilo et al[8]	10 YSZ at 973 K	<768	BMH(parameters adapted from different authors[4,9])	5~25
2004, T. Arima et al[10]	10YSZ at 1000K; 8YSZ at 1200 K, 1400 K, 1600 K	<324	BMH (Brinkman et al)[6]	8~42
2006,Devanathan [11]	6YSZ, 8YSZ at 1125K,1350K; 8YSZ at 1273K	<1500	BMH (Schelling et al)[12]	5.93~25
2010, Araki et aki[13]	4YSZ below 1500K; 4YSZ, 8YSZ at 1600K	<324000	BMH (Brinkman et al[6]; Schelling et al[12])	4, 8, 14
2011, Marrocchelli et al[14]	6.4YSZ at 1250 K; 8.7YSZ at 1670 K	<768	Dipole-polarizable ion model (DIPPIM[15])	5.8-20
2011,Lau and Dunlap[16]	8YSZ at 800 K, 1000 K, 1200 K	<8808	BMH(Lau, Dunlap[16])	3-12
2011, Chang et al[17].	7YSZ at 1273K	<768	BMH(Dwivedi,Cormack[6]; Lewis,C.R.A.Catlow[8])	6-10
2014, Sizov et al[18]	5-7YSZ at 1100-1900K	<1500	BMH(Brinkman et al[6]; Schelling et al[12]; Lau and Dunlap[16])	4-12
2014,Huang et al[19]	4-6YSZ at 1000-1600K	<12000	BMH(Brinkman et al[6])	2-20
2018,Yang et al[20]	9.9YSZ at 1000-1300K; 9.3YSZ at 1400-1500K	96000-4 116 000	BMH (fitted parameters)	8-14.3

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(18) Sizov, V. V.; Lampinen, M. J.; Laaksonen, A. *Solid State Ionics* **2014**, *266*, 29-35.
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Below plots the calculated the diffusion coefficient D over the MD time for 8YSZ at 1400 K. It could be seen that D converges largely after 6 ns, with the value of 0.14×10^{-8} m^2/s, oscillating by $\pm2.8\%$.

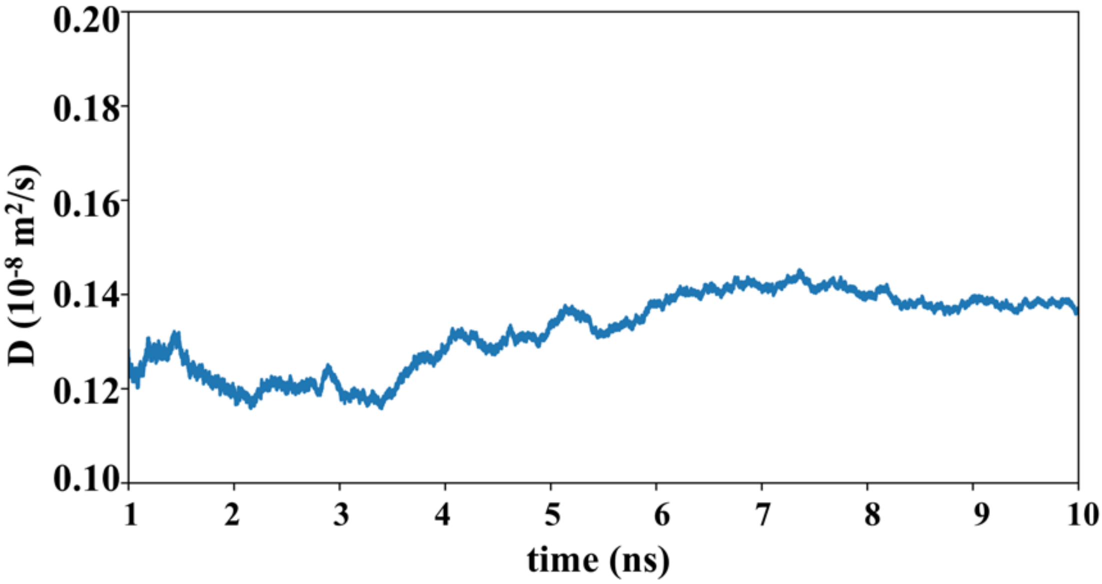

Figure S1. The calculated diffusion coefficients (D) vs simulation time at 1400K for 8YSZ

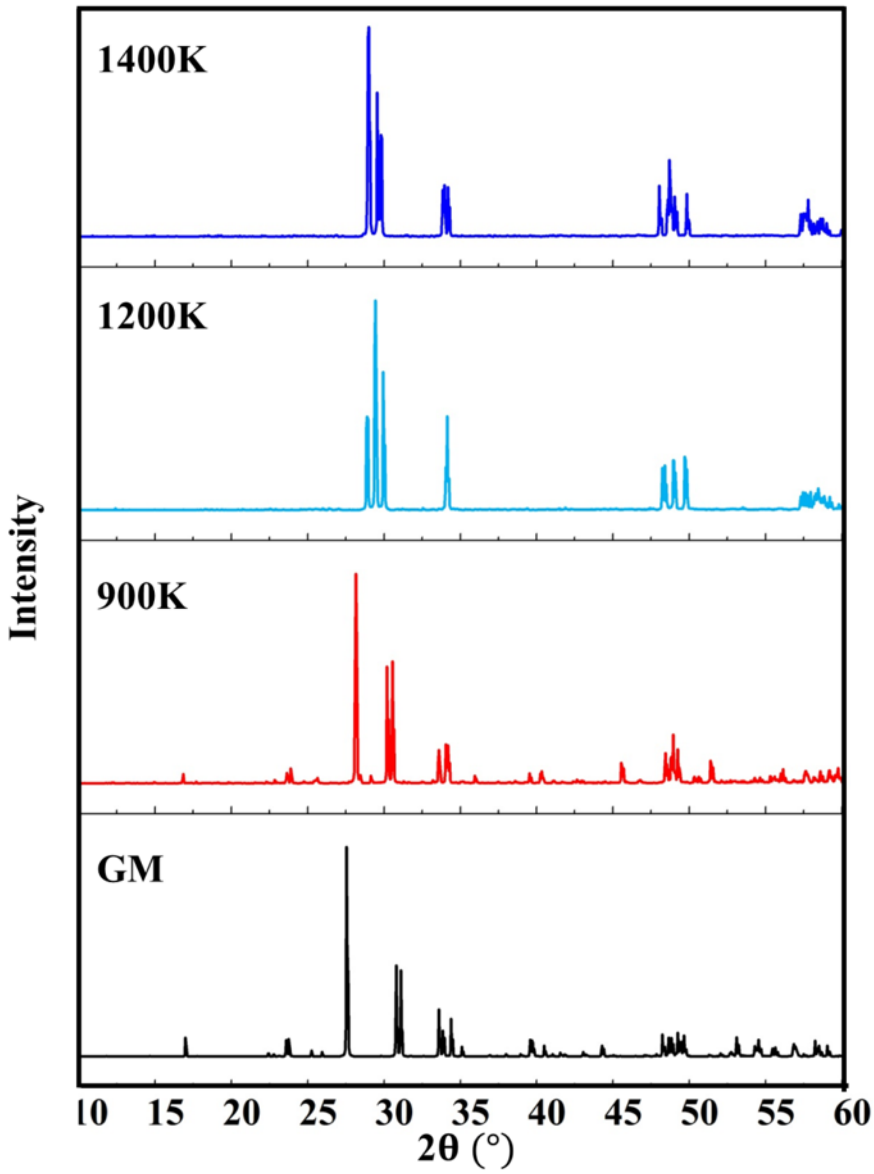

Figure S2. Simulated X-ray diffraction patterns of the 6.7YSZ at different temperatures.

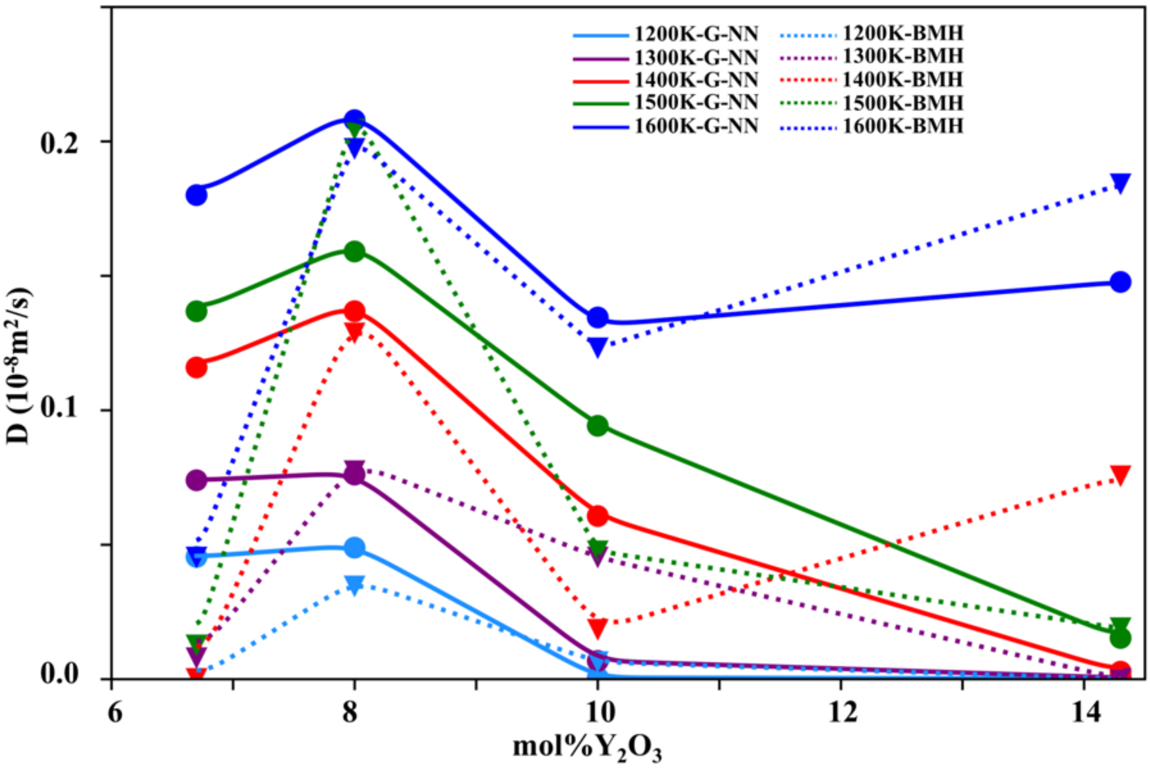

Figure S3. Oxygen diffusion coefficients D vs the Y concentration at different temperatures calculated using empirical BMH potential (dotted line), which are compared with the results from G-NN potential (solid line).

Figure S3 compares the results from empirical BMH potential and G-NN potential results for diffusion coefficient D. It can be seen that the BHM potential is particularly bad for 6.7YSZ, which is monoclinic phase at the GM. In G-NN potential MD simulations 6.7YSZ will have the phase transition from monoclinic to cubic phase the high temperatures, which however doesnot occur in BHM simulations.

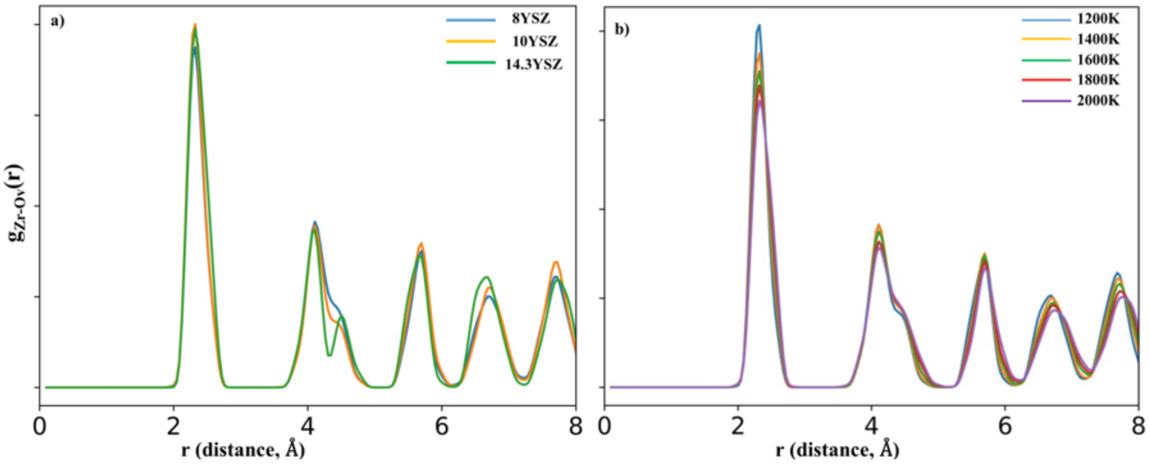

Figure S4. Radial distribution function g(r) of Zr-Ov pairs in 8YSZ, 10YSZ and 14.3YSZ at 1400K (a) and in 8YSZ at different temperatures (b).

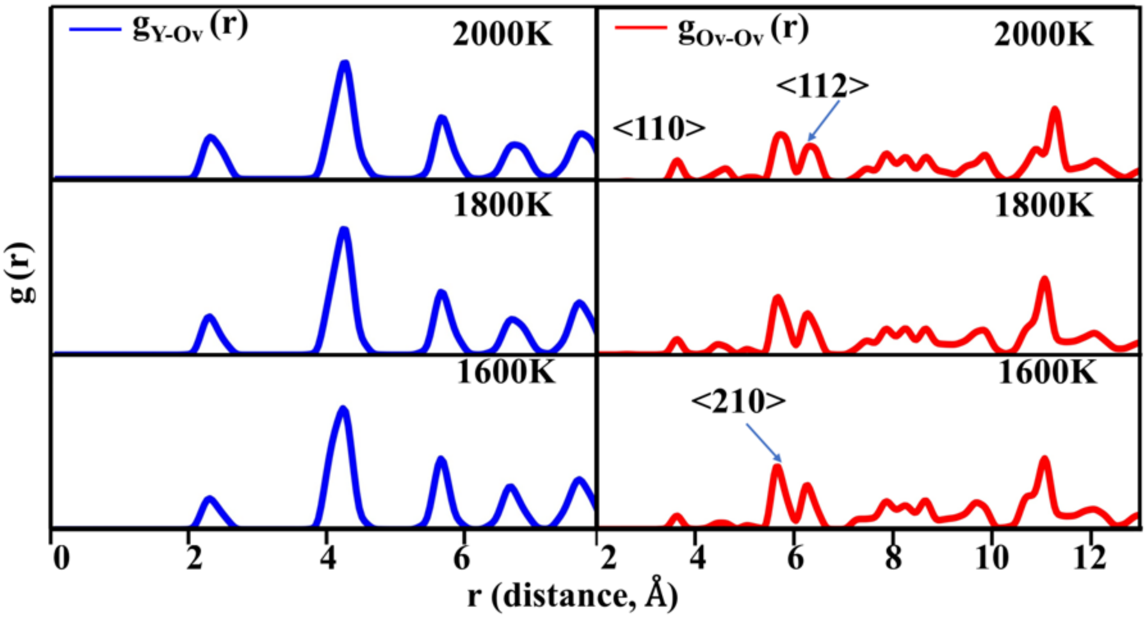

Figure S5. Radial distribution function g(r) of Y-O_v (left panel) and O_v-O_v (right panel) for 8YSZ above 1600 K.

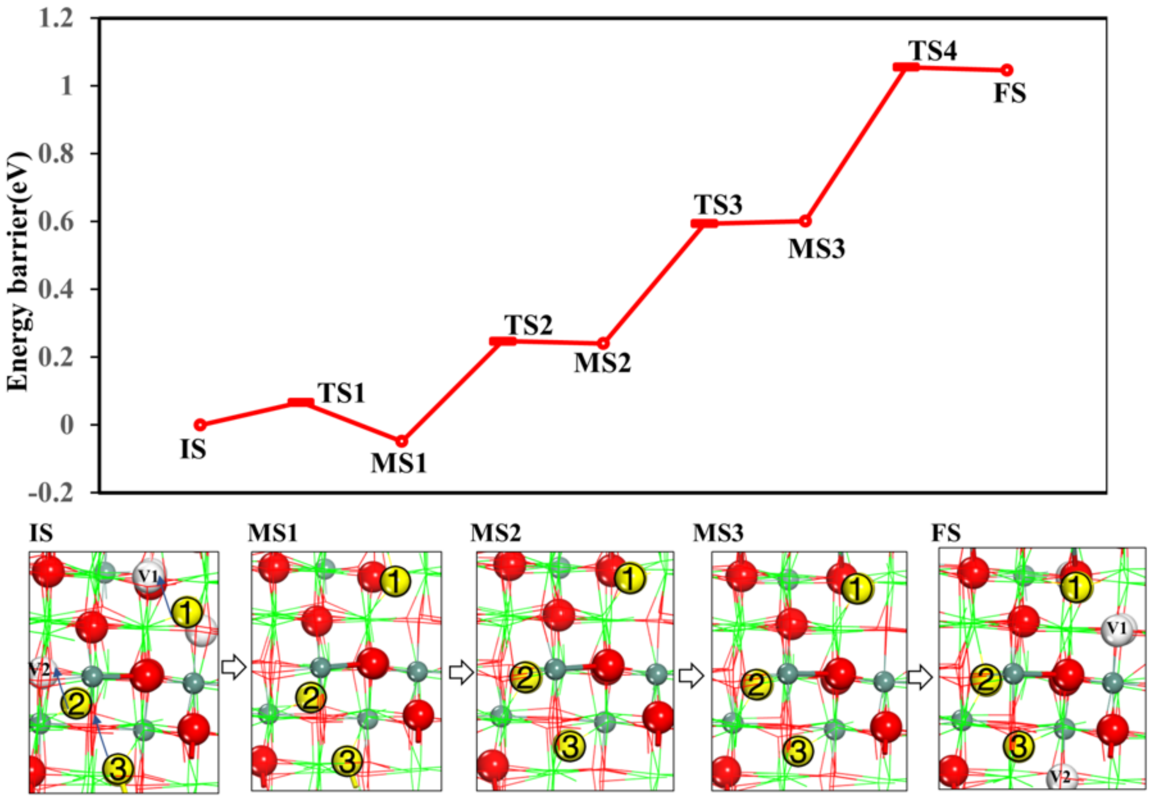

Figure S6. The reaction pathway illustrating how O_v moves in 8YSZ at 1400K. The Euclidean distance of the pathway is 4.74 Å. The reaction energy profile is shown in the top panel and the corresponding structure snapshots along the pathway are shown in the bottom. Y: dark green ball; reacting O: yellow balls with numbers (1,2,3); other resting O: red balls; vacancy: white balls labeled with V1 and V2;