Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for: "Li ion diffusion behavior of Li_3OCl solid-state electrolyte with different defect structures: insights from the deep potential model"

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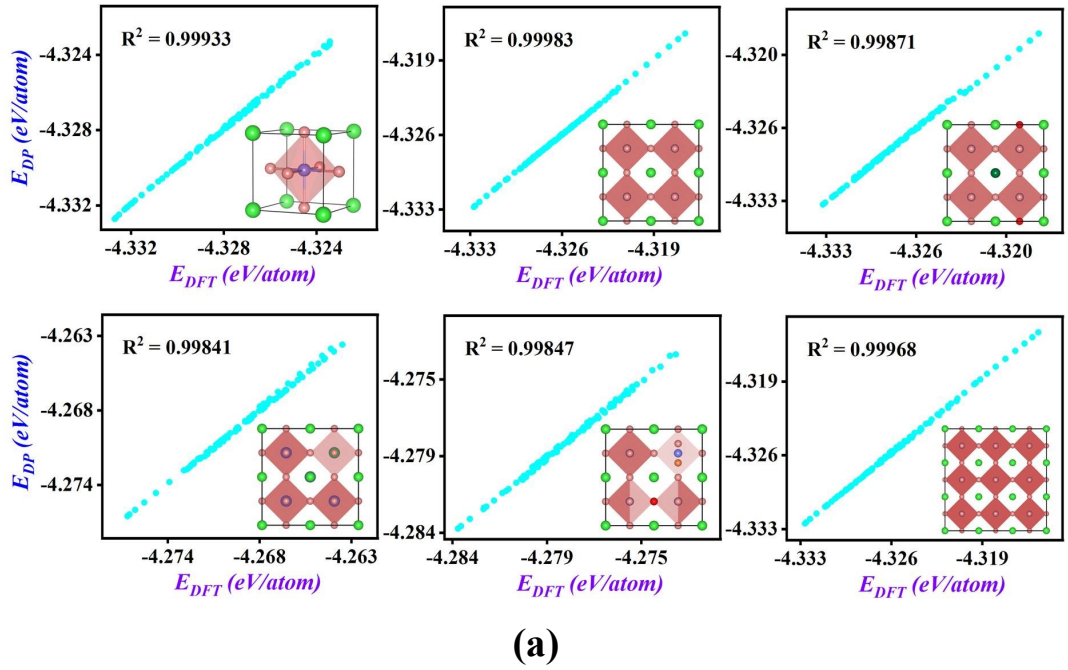
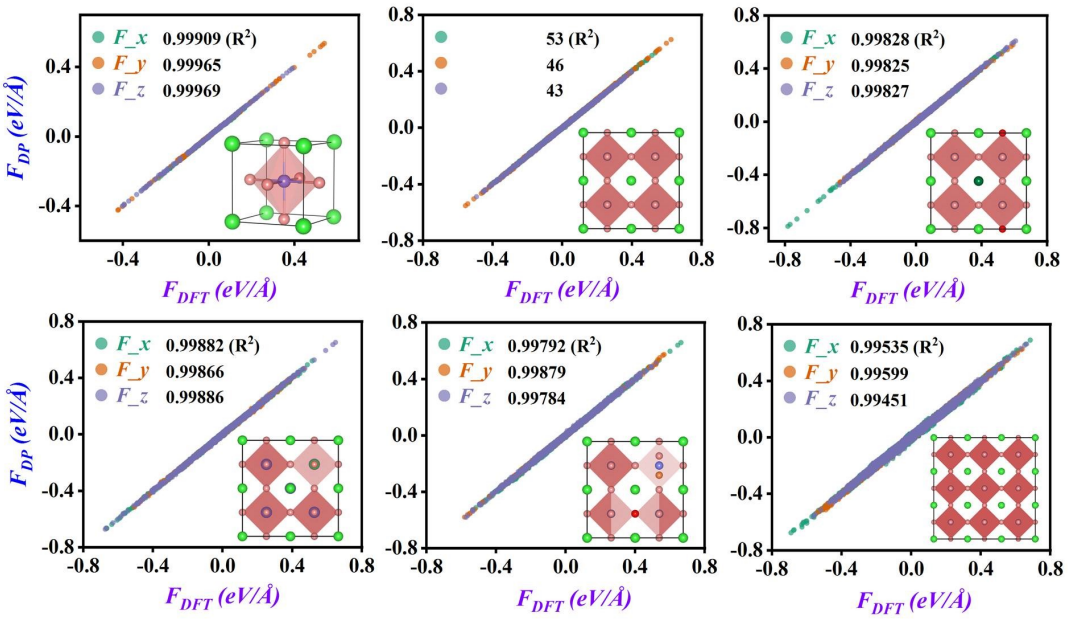
1. Comparison of DP and DFT energy and force calculation results.



(a)



(b)

Figure S1. Plots of energy (a) and force (b) of DP model prediction versus DFT calculation results for each system shown in Figure 1. The coefficient of determination (R^2) for each set of data is given in each panel.

2. MSD curves of different sizes of Li_3OCl systems at different temperatures.

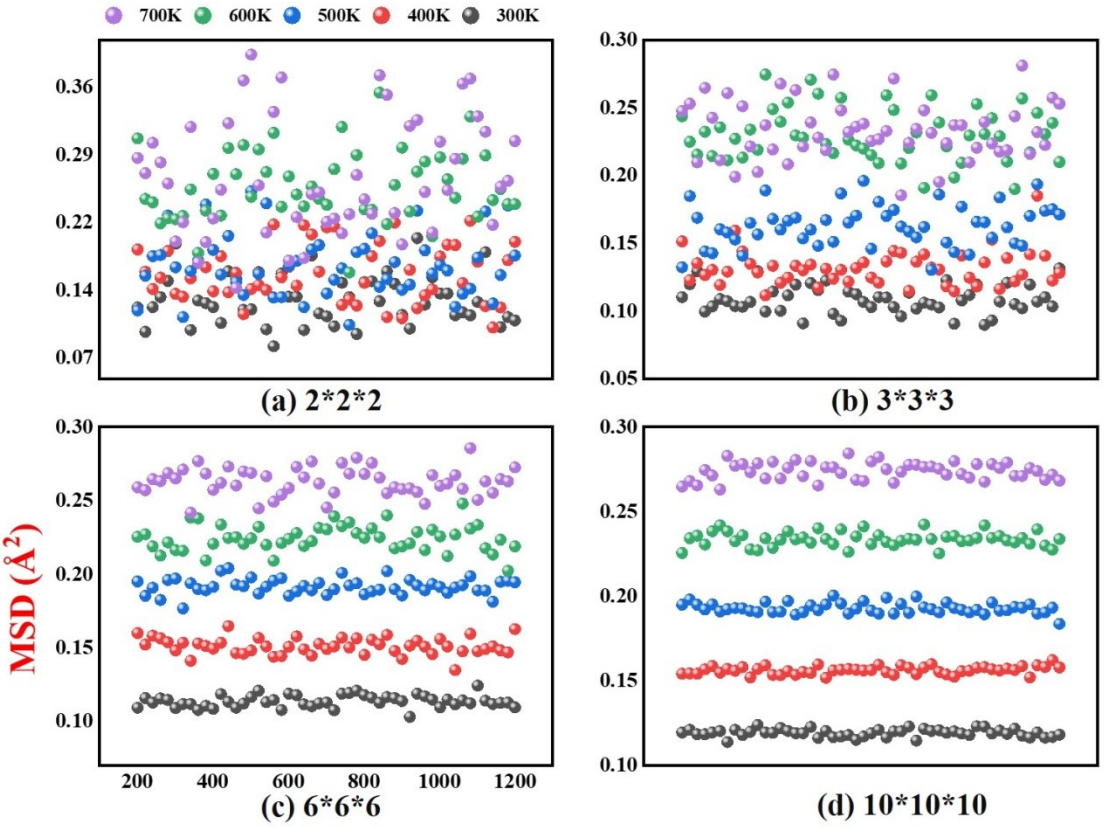


Figure S2. The MSD of Li in four different sizes of perfect crystal structures of with simulation time (Ps) at 300K - 700K.

3. Snapshots of DPMD simulations at different moments in the LiCl-Schottky system at T = 500K. To facilitate the observation of Li migration, each Li atom was labeled with numbers.

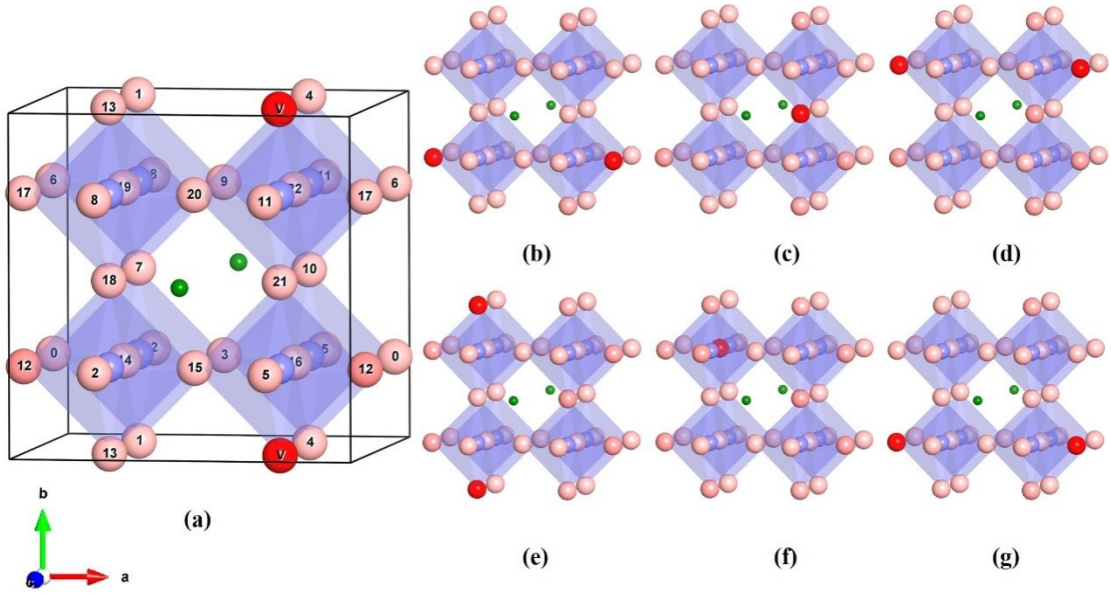


Figure S3. Snapshots of DPMD simulations at different moments in the LiCl-Schottky system. (a) initial structure; (b) energy minimization; (c) 0.3 ns; (d) 0.35 ns; (e) 0.6 ns; (f) 0.8 ns; (g) 1.2 ns. The color scheme is the same as Figure 1. For simplicity, only the positions of the moved vacancy Li atoms (red balls) are displayed, the labels of the other Li ions accompanying the vacancy movements are hidden.

4. MSD curves of (2×2×2) and (10×10×10) LiCl-Schottky defect system at different temperatures.

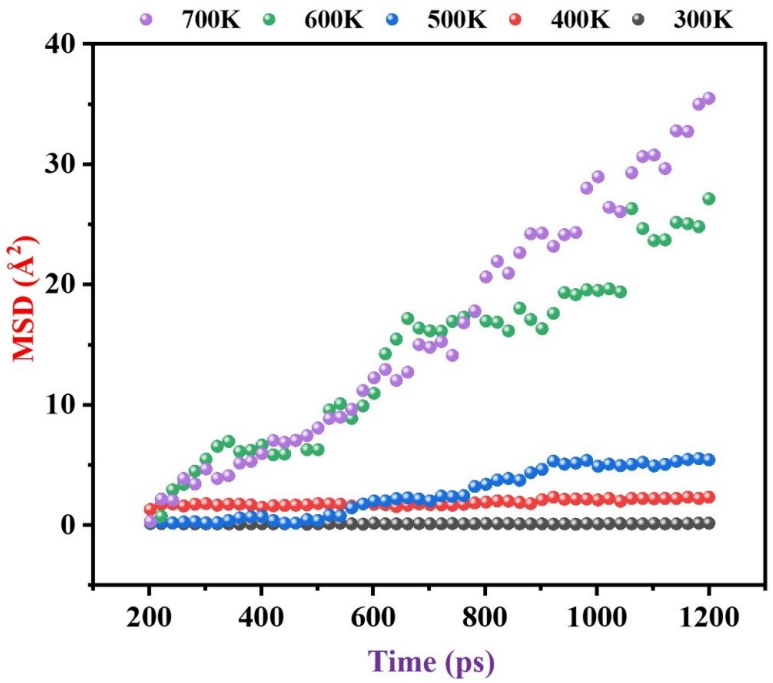


Figure S4. The MSD of Li with simulation time at different temperatures for the (2×2×2) LiCl-Schottky structure.

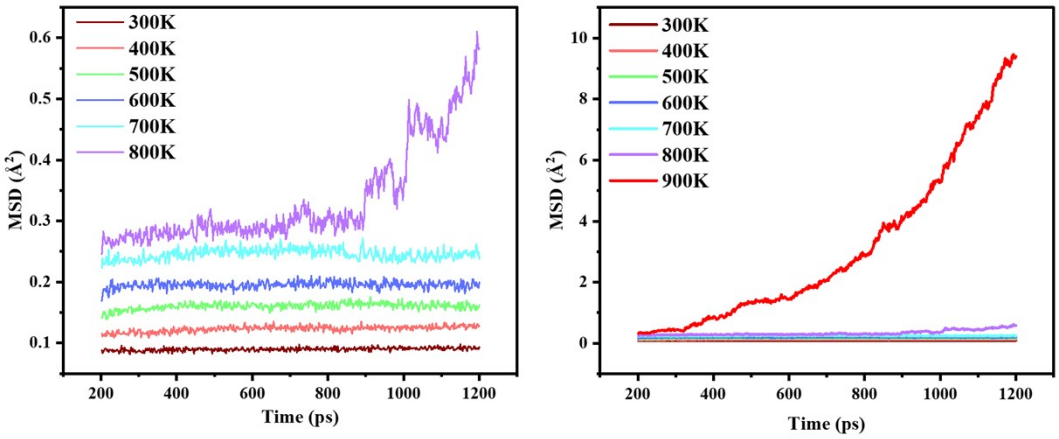


Figure S5. The MSD curves of Cl ions for LiCl-Schottky defect structure with a defect concentration of 12.5% at seven temperature intervals from 300K to 900K.

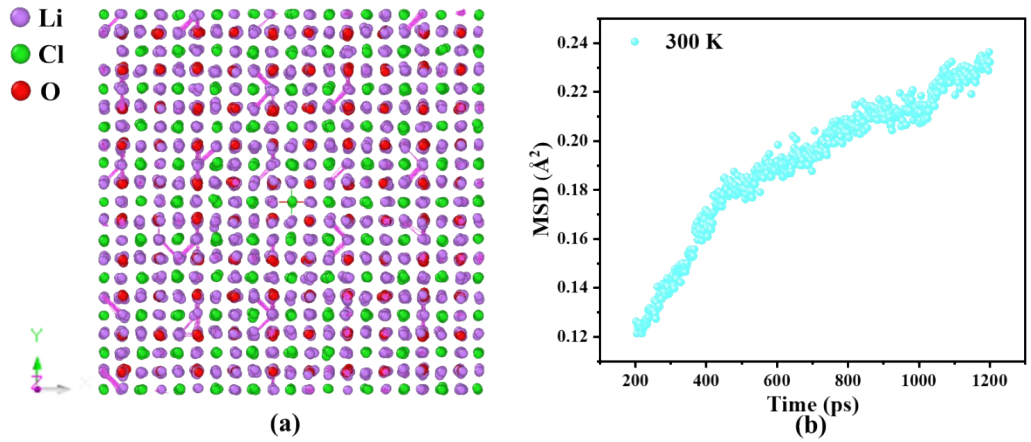


Figure S6. Li ion diffusion trajectory diagram (a) and the MSD curve of Li with simulation time (b) at a temperature of 300 K and a defect concentration of 12.5% in the (10×10×10) LiCl-Schottky defect structure. The purple line in the left panel is the diffusion trajectory line of Li ions.

5. MSD curves of (2×2×2) Li-Frenkel defect system at different temperatures.

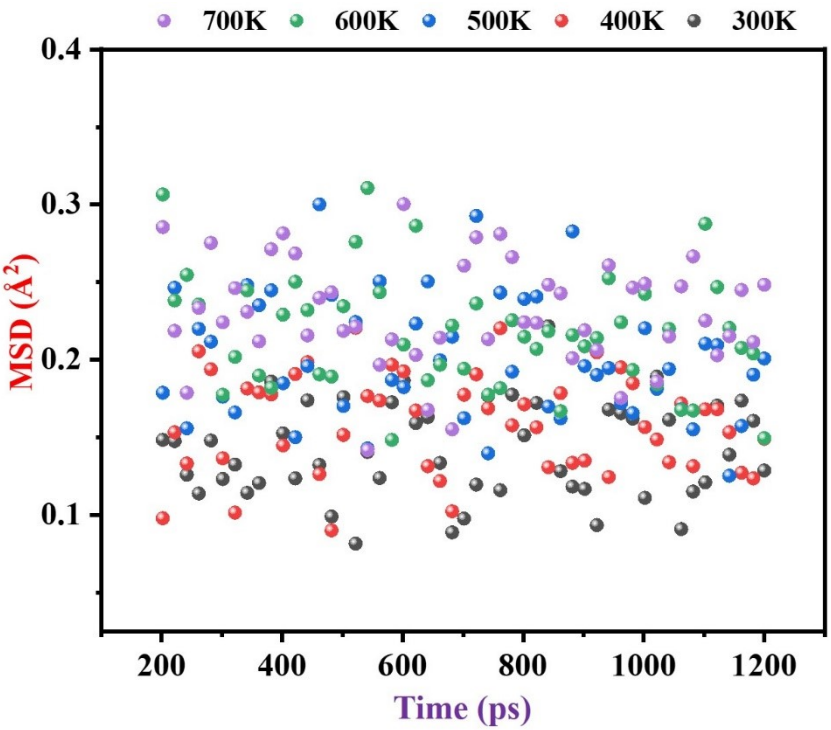


Figure S7. The MSD of Li with simulation time at different temperatures for Li-Frenkel defect structure.

6. Snapshots of DPMD simulations at different moments in the Cl-O anti-site system at T = 700K. The figure only shows the labels of Li atoms that differ from the initial structural position.

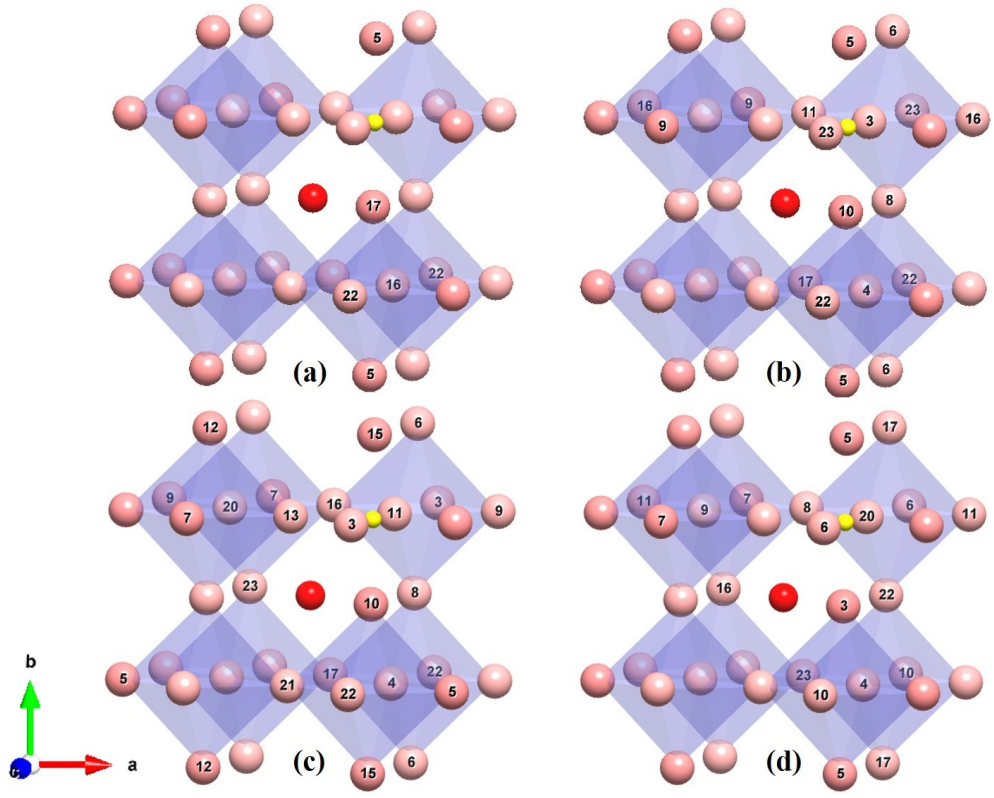


Figure S8. Snapshots of DPMD simulations at different moments in the Cl-O anti-site system at T = 700K. (a) energy minimization; (b) 0.4 ns; (c) 0.8 ns; (g) 1.2 ns. Yellow and red atoms represent $Cl_O^{\bullet}$ and $O_{Cl}^{'}$ respectively.

7. MSD curves of (2×2×2) Cl-O anti-site disordered system at different temperatures.

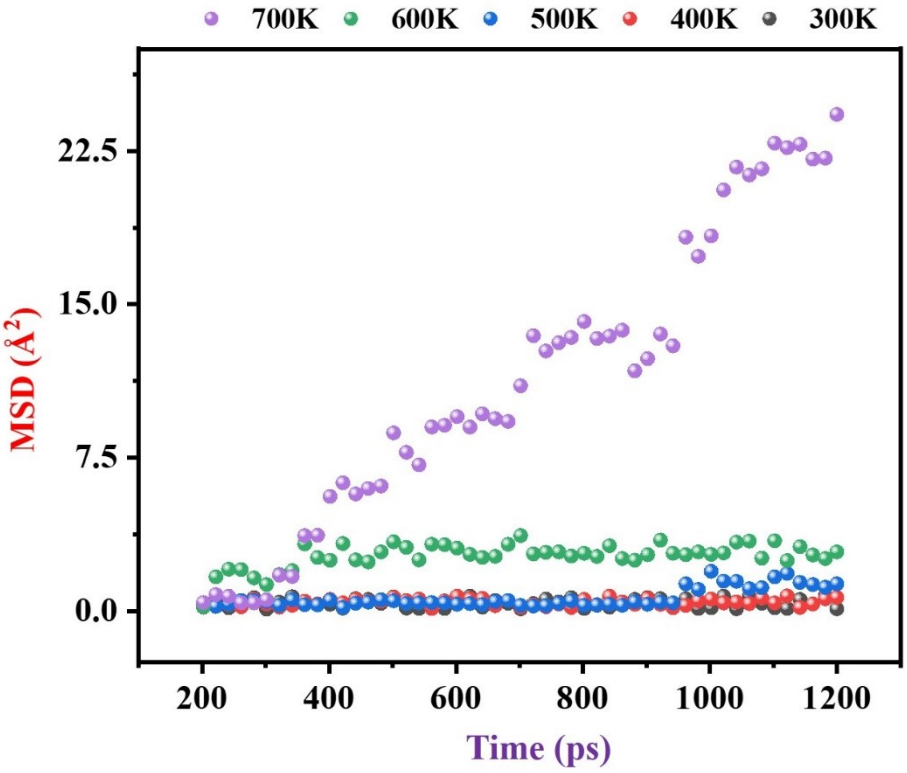


Figure S9. The MSD of Li with simulation time at different temperatures for Cl-O anti-site disordered system.

8. MSD curves and diffusion coefficient results of (10×10×10) Cl-O anti-site disordered system at different temperatures.

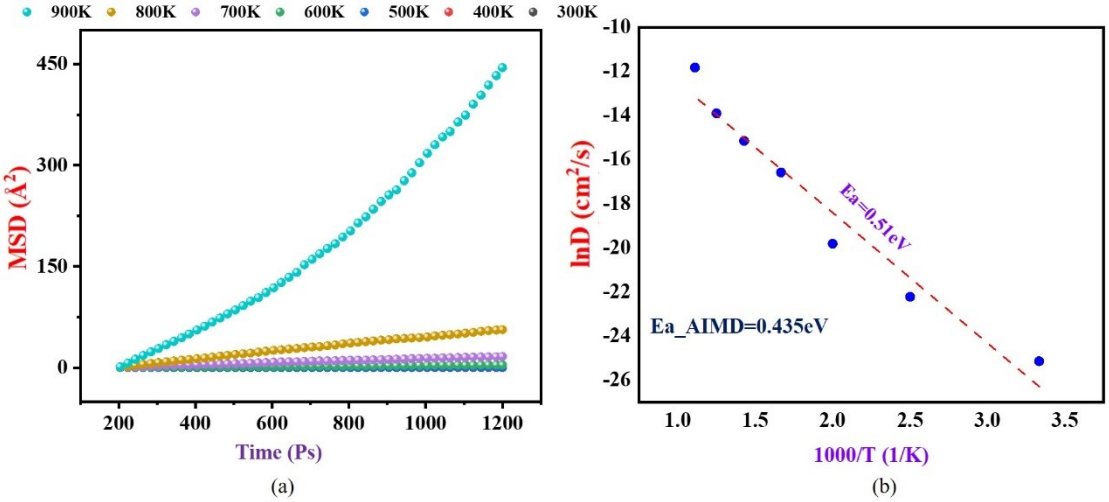


Figure S10. Diffusion properties in the (10×10×10) Cl-O anti-site disorder system. (a) MSD of Li at different temperatures with time. (b) The diffusion coefficient and the activation energy results of the system.

9. Comparison of ionic conductivity between different structures in Li_3OCl system.

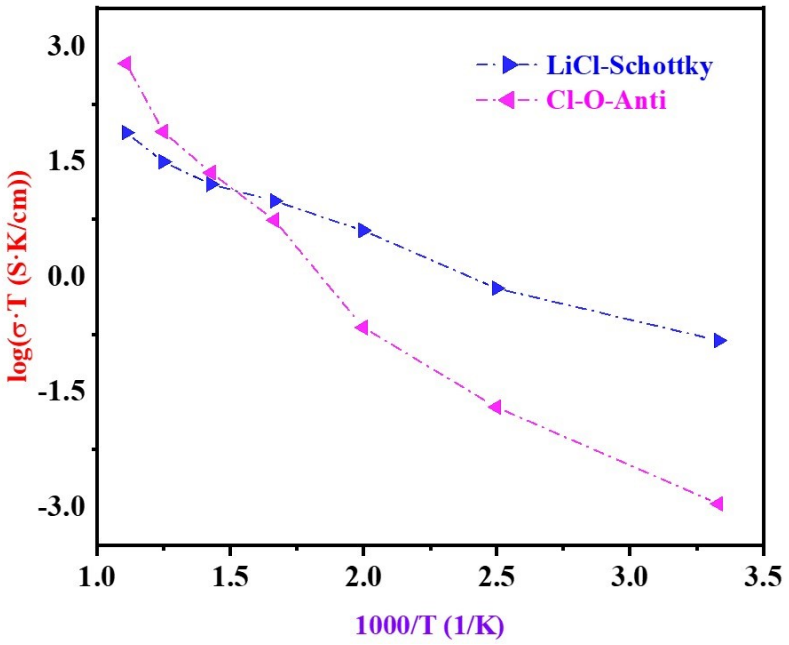


Figure S11. Comparison of the ionic conductivity between the LiCl-Schottky defect and anti-disorder structures in Li_3OCl system at different temperatures.

10. Activation energy of different defect concentration LiCl-Schottky systems.

Table S1. Activation energy of different defect concentration systems

$Li_{3-x}OCl_{1-x}$	E_a (eV)
x = 5%	0.276
x = 7.5%	0.243
x = 12.5%	0.239