

SUPPLEMENTARY MATERIAL

Unveiling the structure and ions dynamics of amorphous $\text{Na}_{3-x}\text{OH}_x\text{Cl}$ antiperovskite electrolytes by first-principles molecular dynamics[†]

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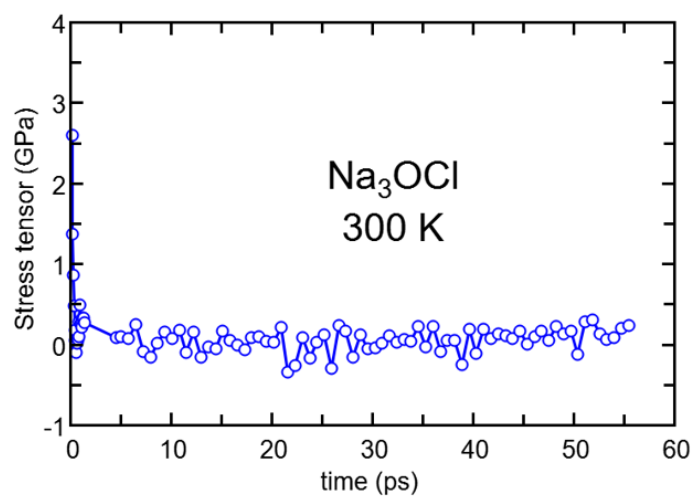


Fig. S1 (Color online) Stress tensor data vs time of Na₃OCl model at 300 K, reported as average of the diagonal components.

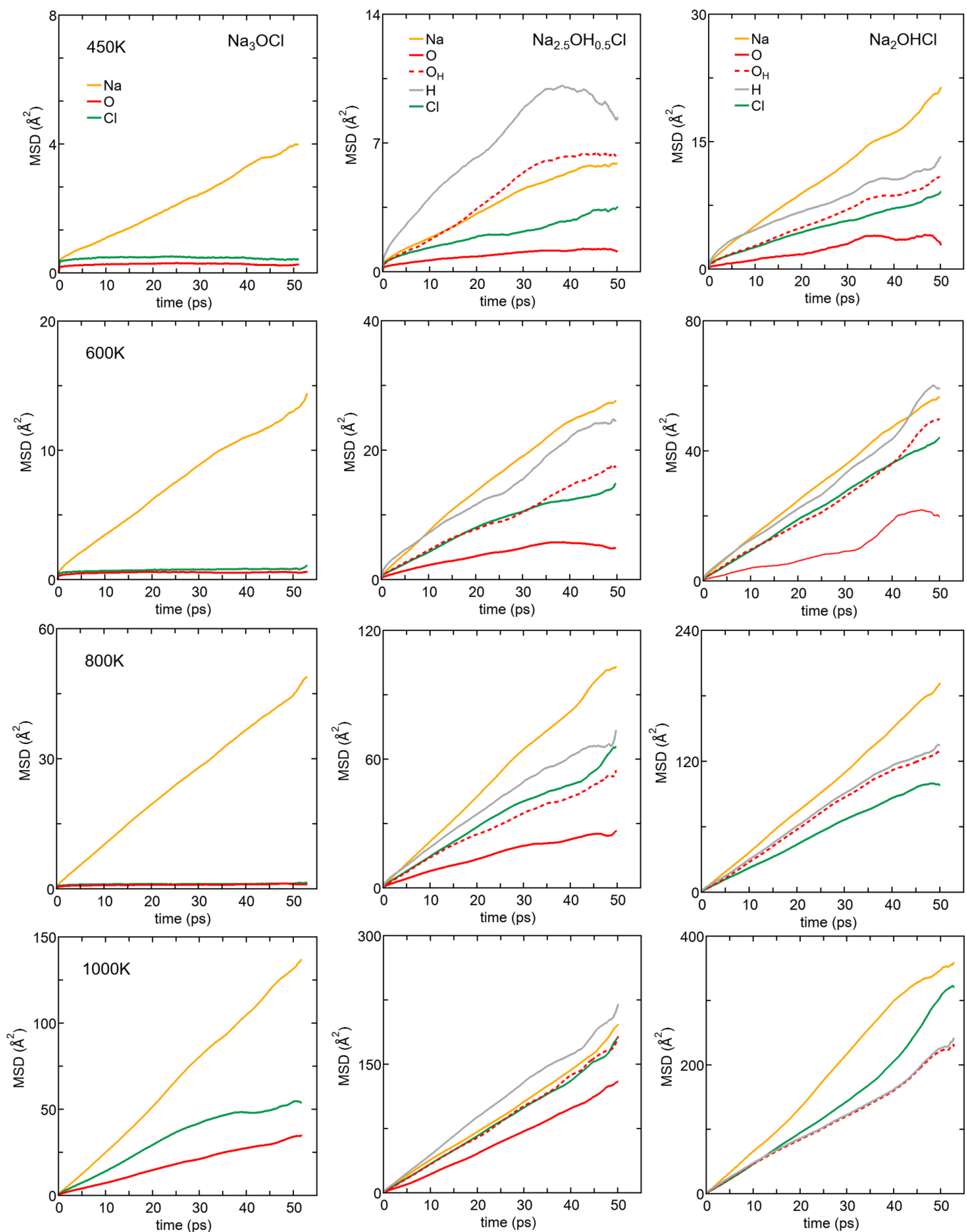


Fig. S2 (Color online) MSD vs time for each element in $\text{Na}_{3-x}\text{OH}_x\text{Cl}$ systems at 450 K, 600 K, 800 K, and 1000 K. Colors legend: Na, yellow; O non bonded to H atoms, red (solid line); O bonded to H atoms, red (dashed line); H, grey; Cl, green.

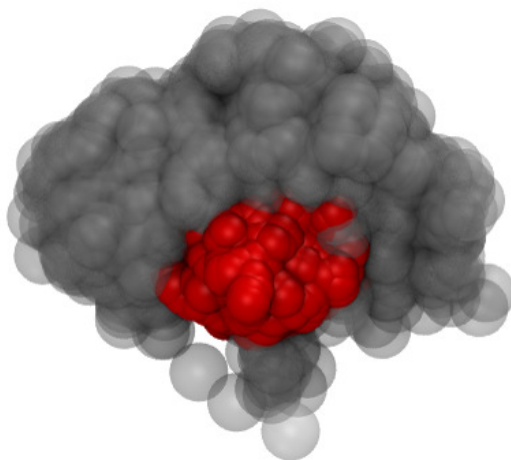


Fig. S3 (Color online) Rotational dynamical disorder of a given H atom (grey transparent sphere) around one O atom (red opaque sphere) of one hydroxyl OH group in amorphous $\text{Na}_{2.5}\text{OH}_{0.5}\text{Cl}$ over a time span of ~ 50 ps.

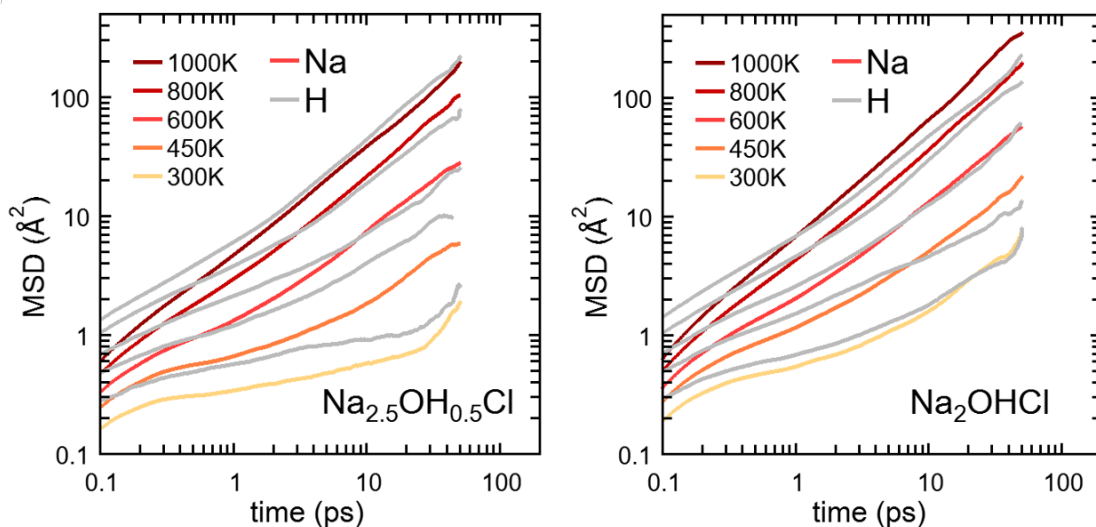


Fig. S4 (Color online) Log-log plot of MSD vs time for Na and H atoms in between 300 K and 1000 K for $\text{Na}_{2.5}\text{OH}_{0.5}\text{Cl}$ (left) and Na_2OHCl (right).

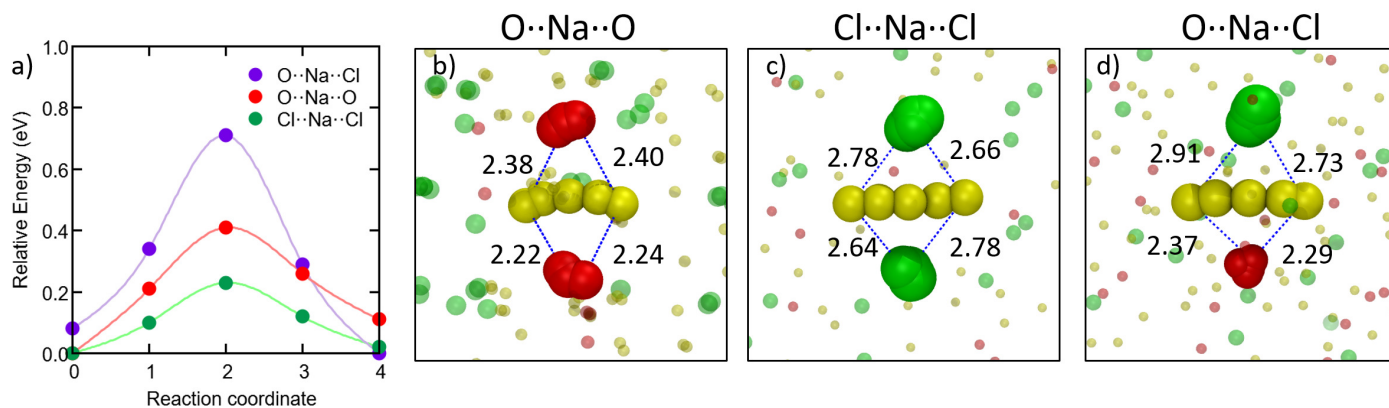


Fig. S5 (Color online) a) Transition state minimum-energy path calculations of Na migration through two atom pairs for Na_3OCl at 300 K. We show the corresponding images configurations for Na migrating through two O atoms (b), two Cl (c), and a O and a Cl atoms (d). The initial and final bond distances are indicated in Å.