Supplementary Information

A First Principle Study of the Phase Stability, Ion Transport and Substitution Strategy for Highly Ionic Conductive Sodium Antipervoskite as Solid Electrolyte for Sodium Ion Batteries

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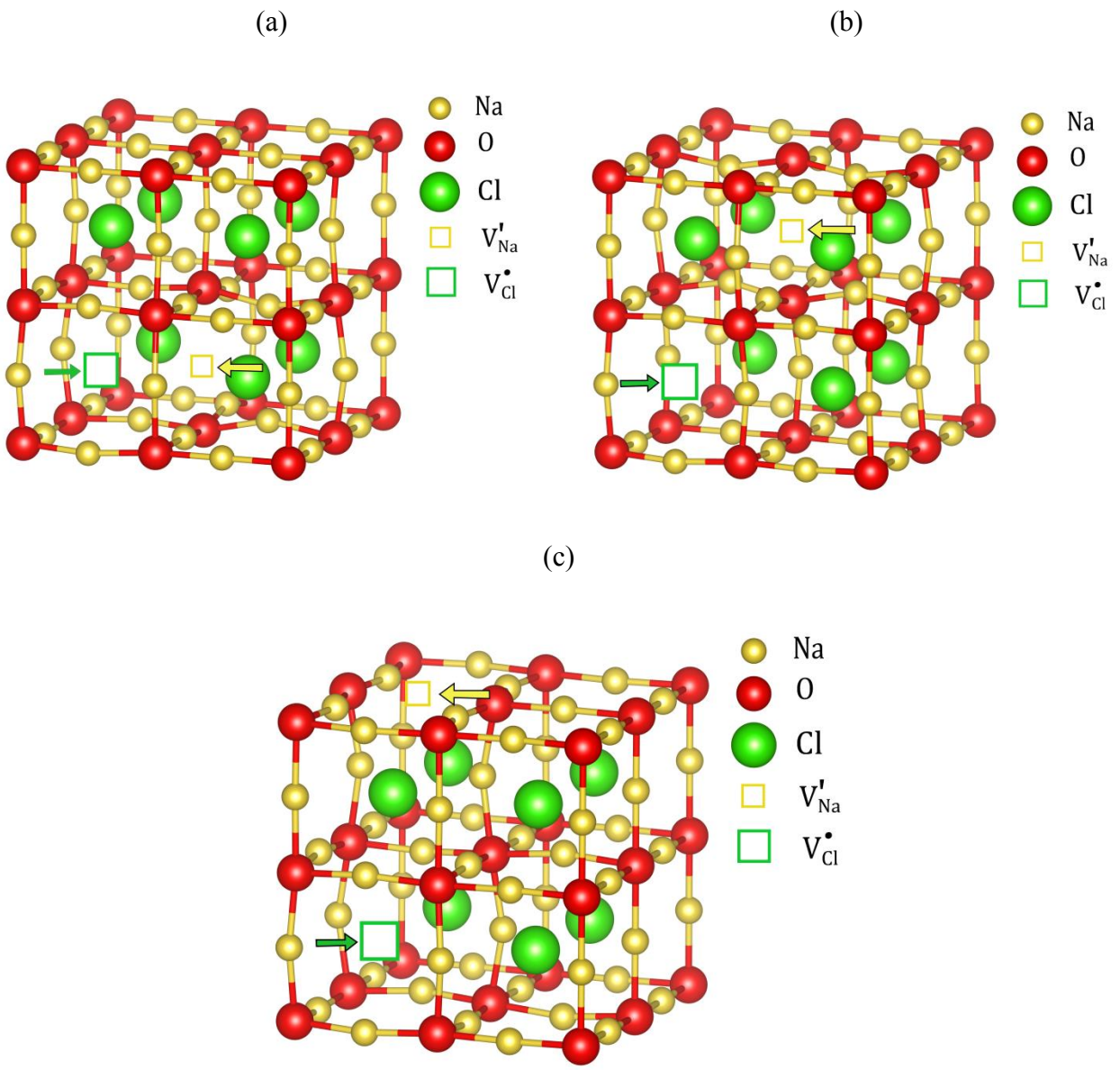


Figure S 1 The three lowest energy configurations for the NaCl Schottky defect pair,(a) NN, (b) 2NN and (c) 3NN configuration. Yellow square denotes V'_{Na}, green square denotes $V^{\bullet}_{Cl}$. The computed defect formation energy are given in Table 1 of the main text. (For the sake of illustration, $2 \times 2 \times 2$ supercell is shown instead of the $3 \times 3 \times 3$ supercell).

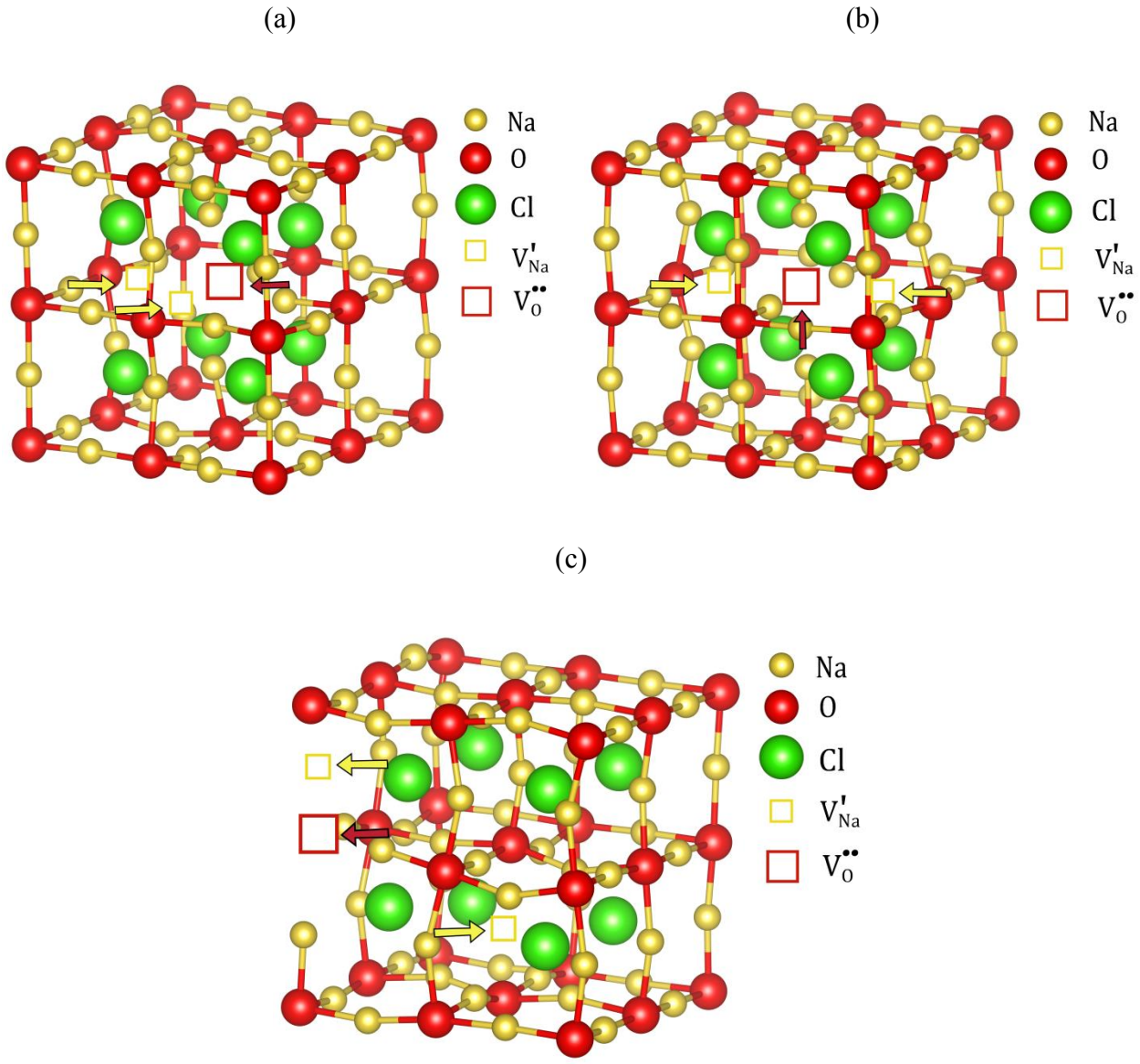


Figure S 2 The three lowest energy configuration for Na_2O Schottky defect pair, (a) adjacent, (b) opposite, and (c) Separated configuration. Spheres with yellow frame denote V'_{Na} and spheres with red frame denote $V_O^{\bullet\bullet}$. The computed defect formation energy are given in Table 1 of the main text. (For the sake of illustration, $2 \times 2 \times 2$ supercell is shown instead of the $3 \times 3 \times 3$ supercell).

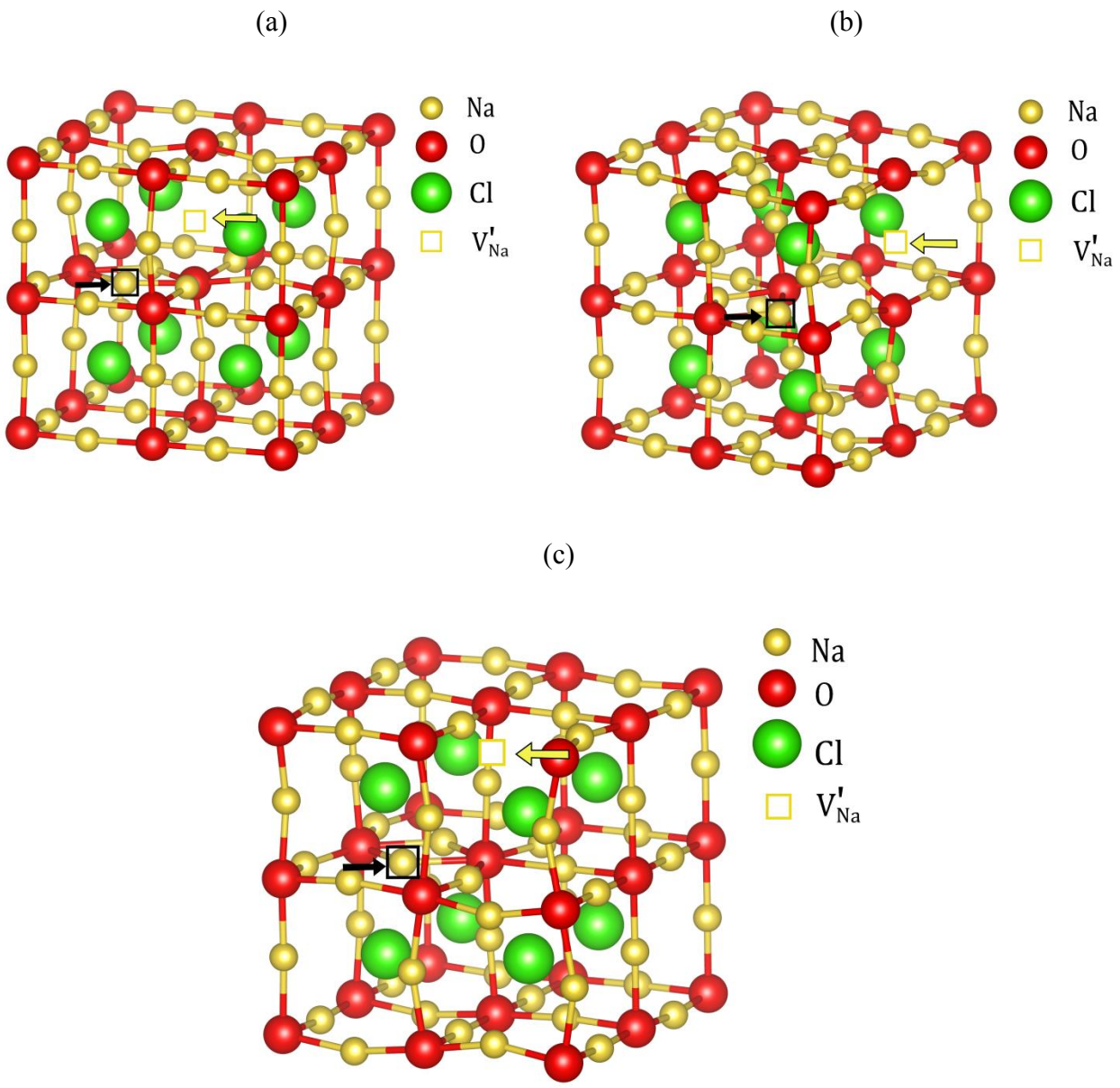


Figure S 3 The three lowest energy configurations being considered for Na Frenkel defect pair, (a) NN, (b) 2NN, and (c) 3NN configuration. Spheres with yellow frame denote V'_{Na}, the black frame mark the position of $Na_i^{\bullet}$. The computed defect formation energy are given in Table 1 of the main text. (For the sake of illustration, $2 \times 2 \times 2$ supercell is shown instead of the $3 \times 3 \times 3$ supercell).

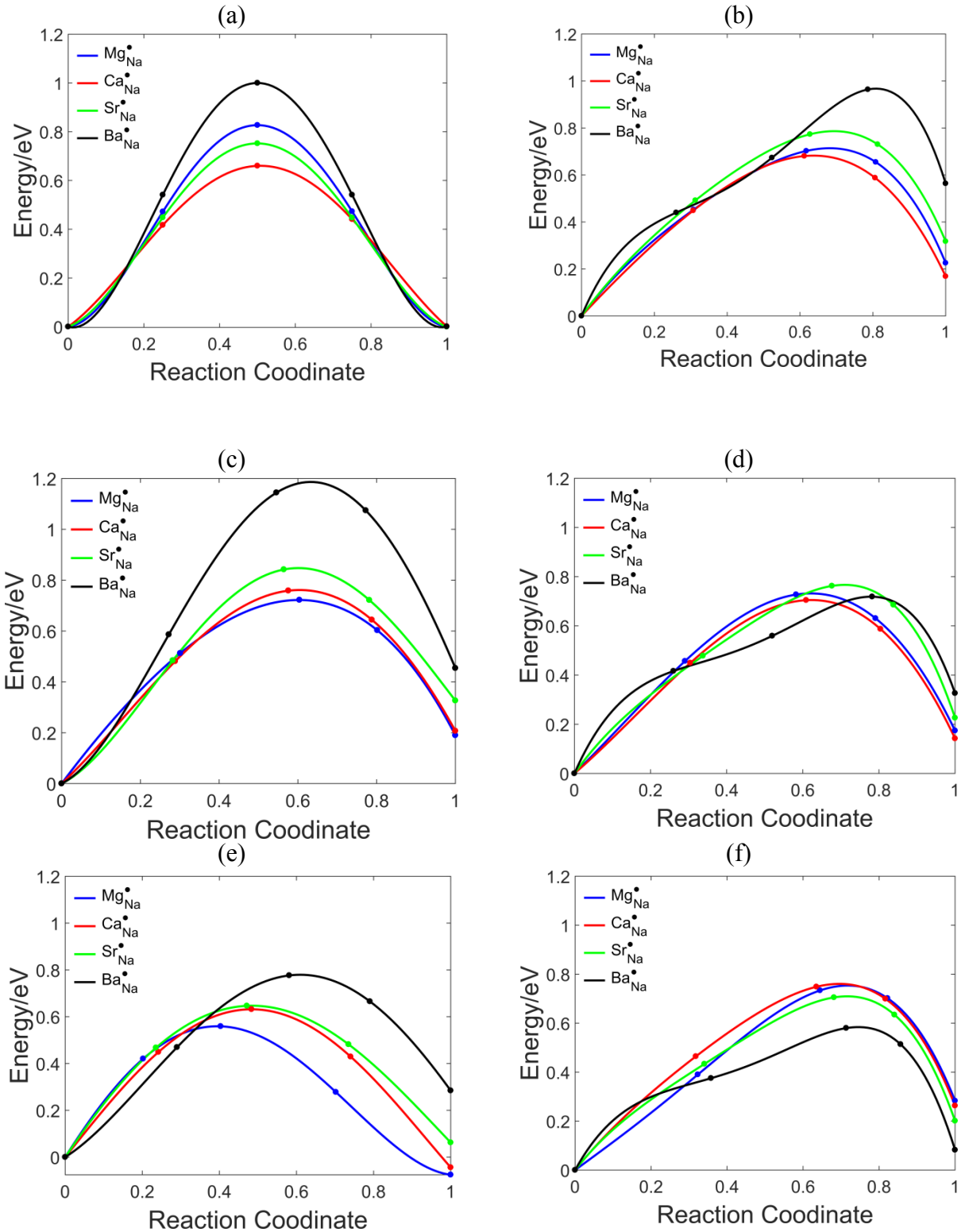
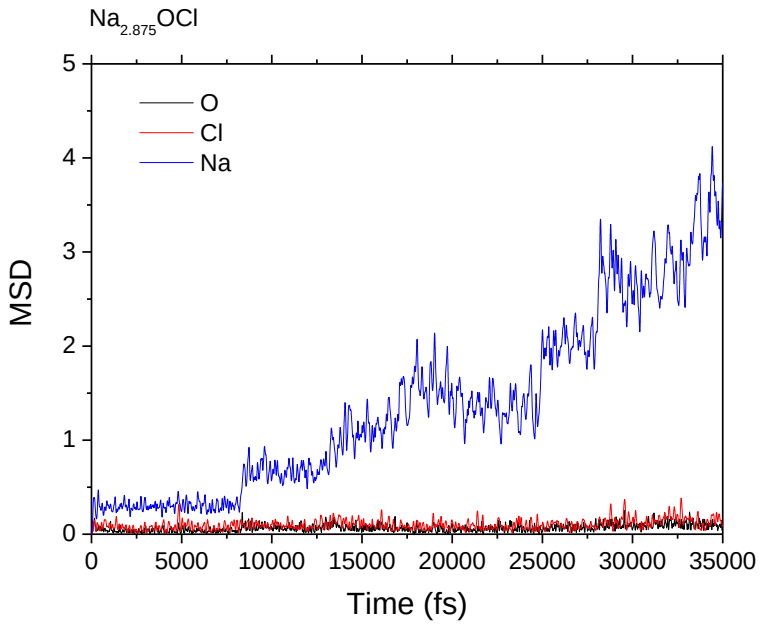


Figure S 4 Energy-reaction coordinate as obtained from NEB calculation. Panel (a)-(f) shows the reaction coordinates for path 1-6.

(a)



(b)

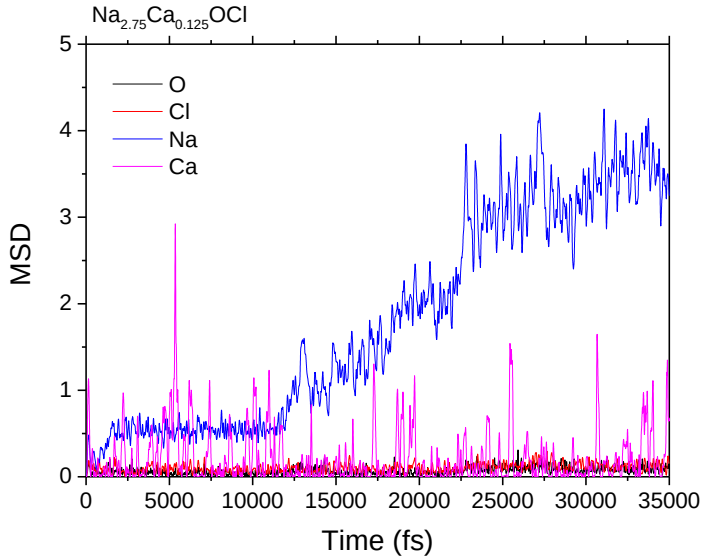
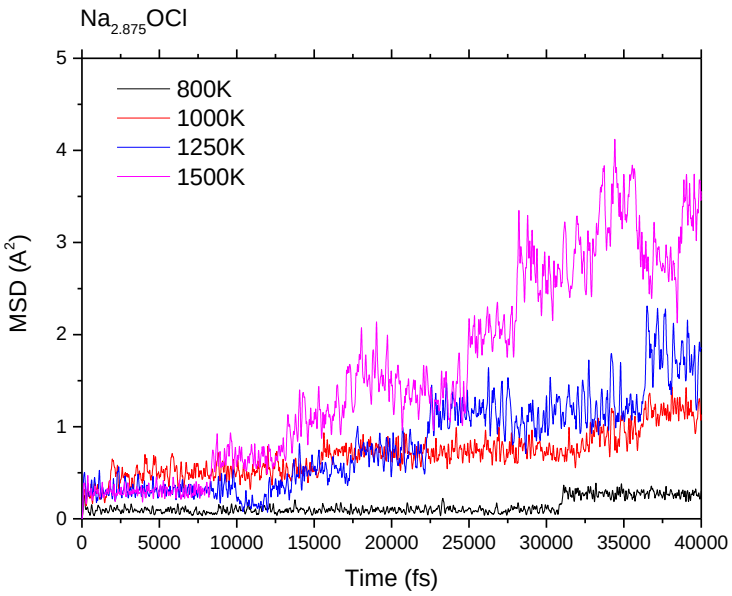


Figure S 5 The mean square displacement of the AIMD simulation for (a) $Na_{2.875}OCl$, and (b $Na_{2.75}Ca_{0.125}OCl$ at 1500K

(a)



(b)

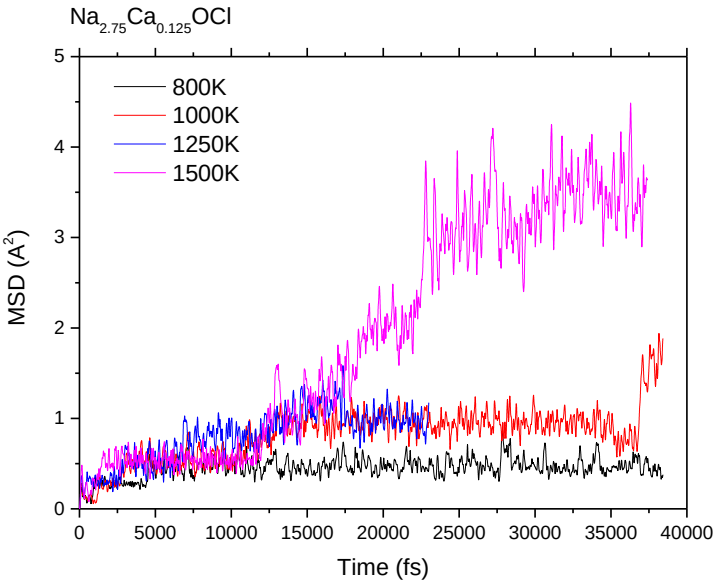


Figure S 6 The mean square displacement of Na ion of the AIMD simulation for (a) $Na_{2.875}OCl$, and (b) the $Na_{2.75}Ca_{0.125}OCl$ at various temperature.