Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

Ab-initio Investigations of Orthogonal ScC_2 and ScN_2 Monolayers as Promising Anode Materials for Sodium-Ion Batteries

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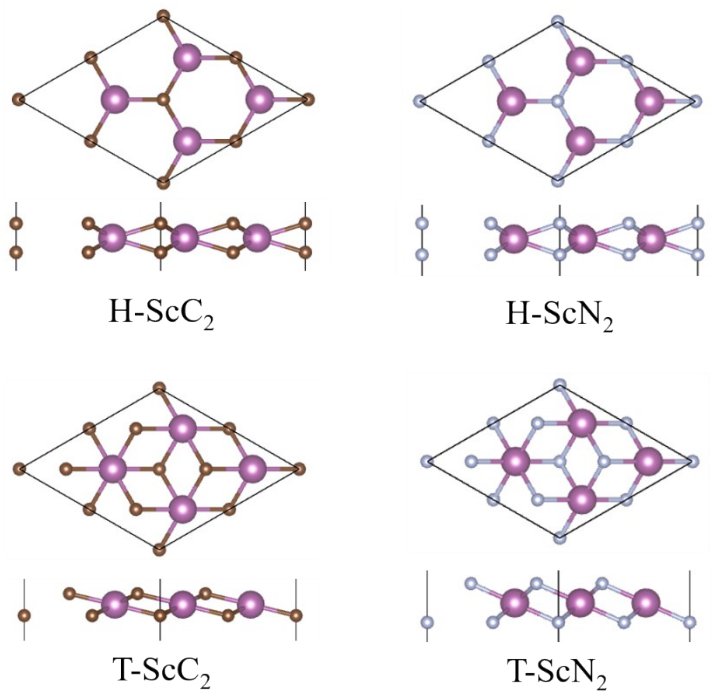

Figure S1. Optimized configurations of the H phases and T phases of ScC_2 and ScN_2 2×2×1 supercell with the top and side perspective. The purple balls represent Sc atoms, brown ones represent C atoms, and white ones represent N atoms.

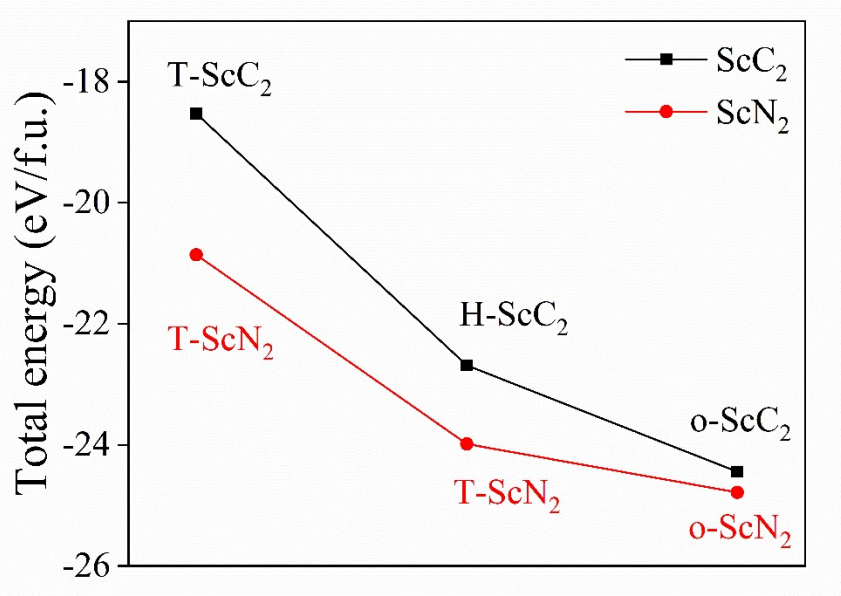

Figure S2. The calculated total energies of T phases, H phases and orthogonal phases of ScC_2 and ScN_2.

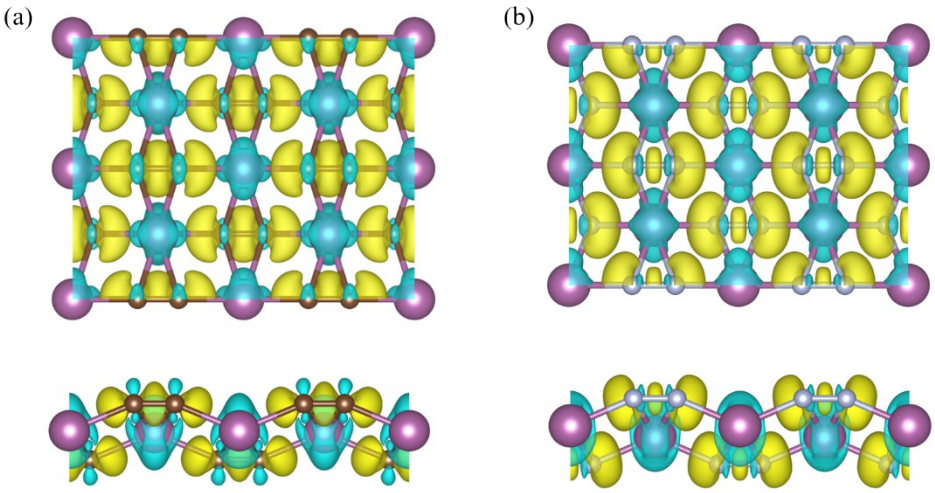

Figure S3. Charge density difference of the (a) o-ScC_2 and (b) o-ScN_2 monolayers with an isovalue of 0.01 e/Bohr^3 calculated by Equation 1. The yellow regions mean electron accumulation and blue ones mean electron depletion. The purple balls represent Sc atoms, brown ones represent C atoms, and white ones represent N atoms.

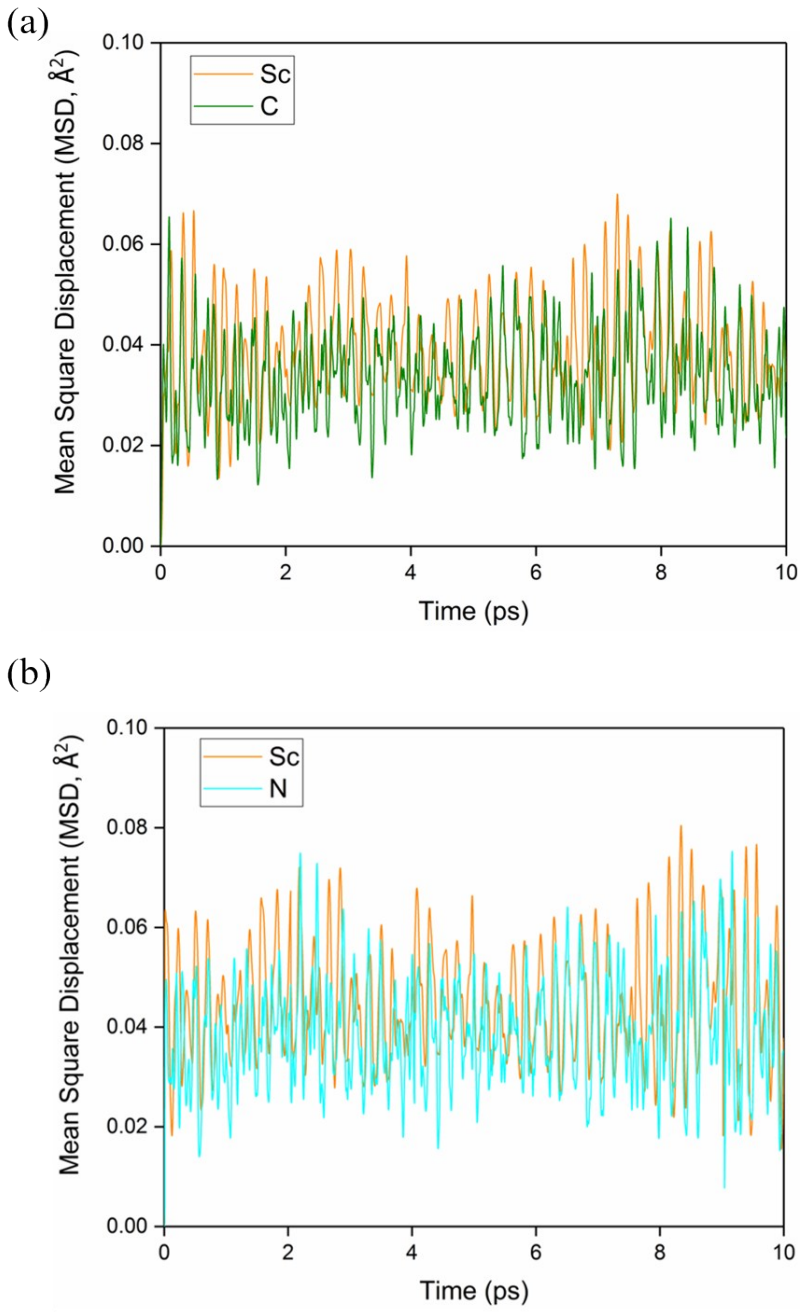

Figure S4. Total mean square displacement (MSD) of the (a) o-ScC_2 and (b) o-ScN_2 $3 \times 3 \times 1$ supercells with a 10 ps duration by the *ab-initio* MD simulation at 300 K.

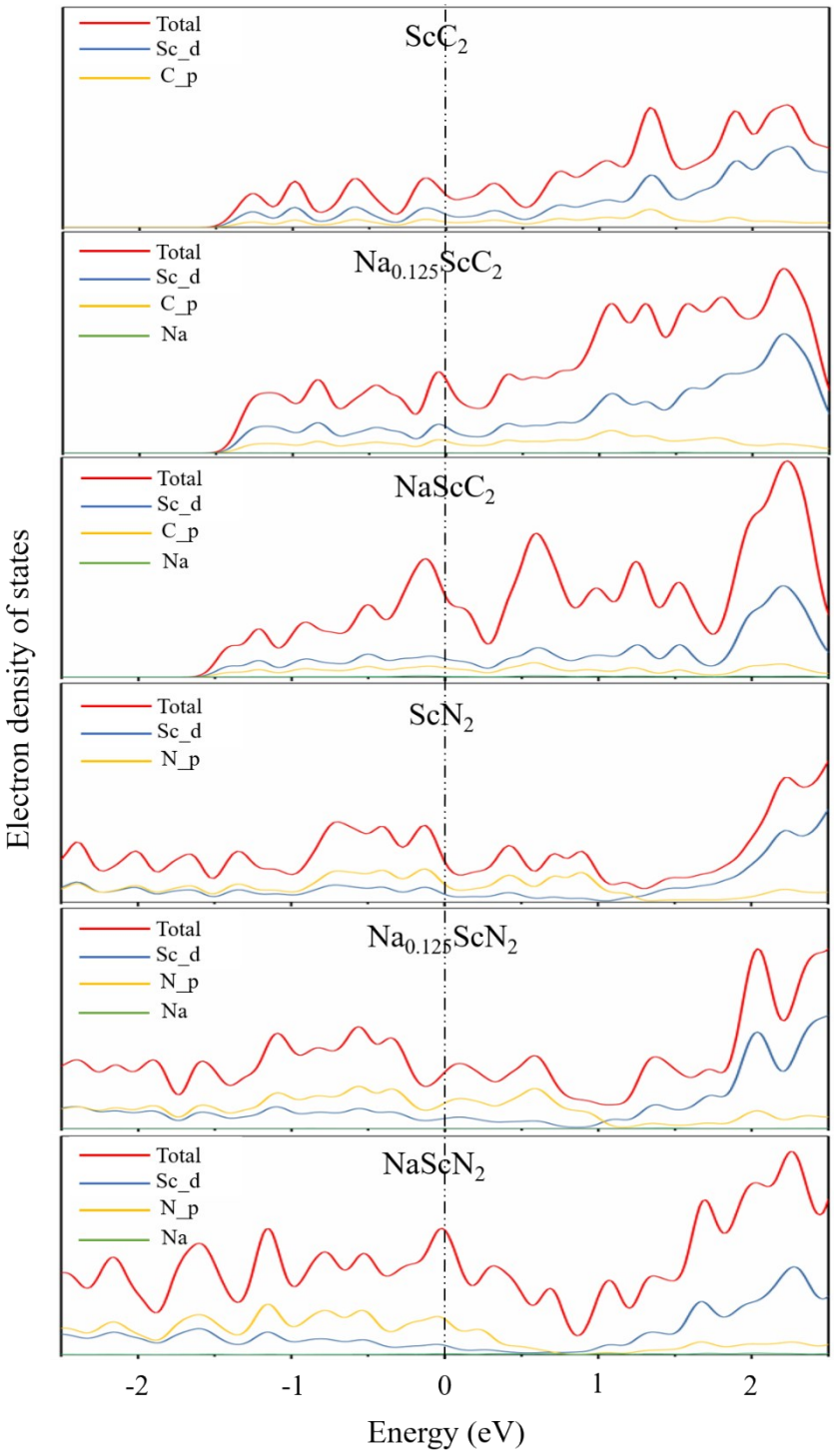

Figure S5. Partial electron density of states of $ScC_2/Na_{0.125}ScC_2/NaScC_2$ and $ScC_2/Na_{0.125}ScC_2/NaScC_2$, respectively. The Fermi energy level is set to zero energy, marked with the black dotted lines.

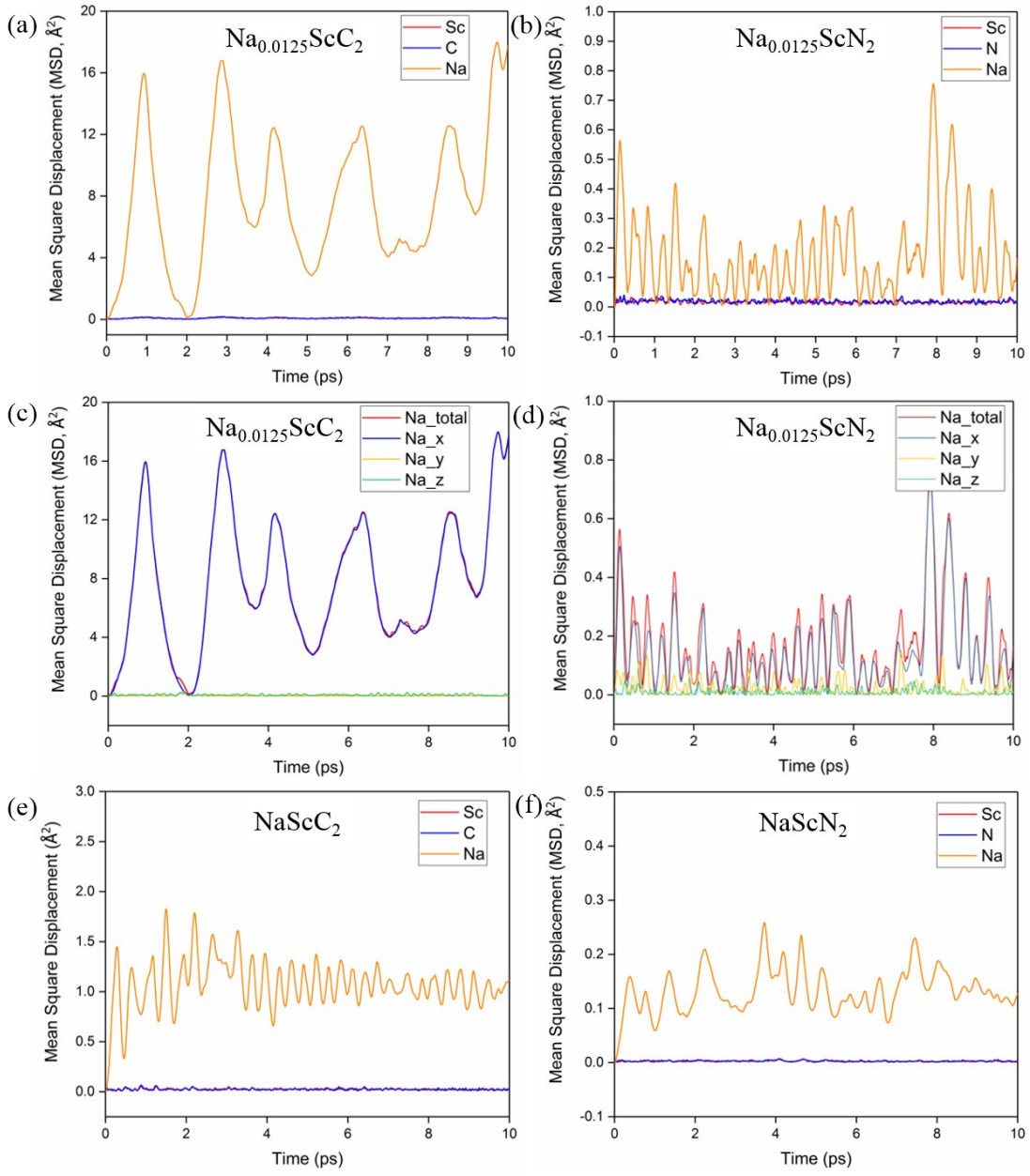

Figure S6. (a) and (b) show the mean square displacements (MSD) of all atoms in o-$Na_{0.0125}ScC_2$ and o-$Na_{0.0125}ScN_2$ monolayers at 300 K. It is clearly demonstrated that energy barrier for Na ion diffusion on o-ScC_2 monolayer is much lower than that on o-ScN_2 monolayer because of over 40 times higher MSD value of Na ions (orange line). (c) and (d) decompose the MSD of Na ion got from (a) and (b). It is observed that MSD value of Na ions is mostly attributed by the Na ion diffusion along the x direction, which is corresponding to the Path 2, the most favourable pathway for Na ion diffusion on the o-ScC_2 and o-ScN_2 monolayers. (e) and (f) show the MSD of o-$NaScC_2$

and o-$NaScN_2$ monolayers with a relatively high Na ion concentration. All AIMD simulations prove the thermodynamic stability of both o-ScC_2 and o-ScN_2 monolayers with low and high concentration Na ion adsorption.

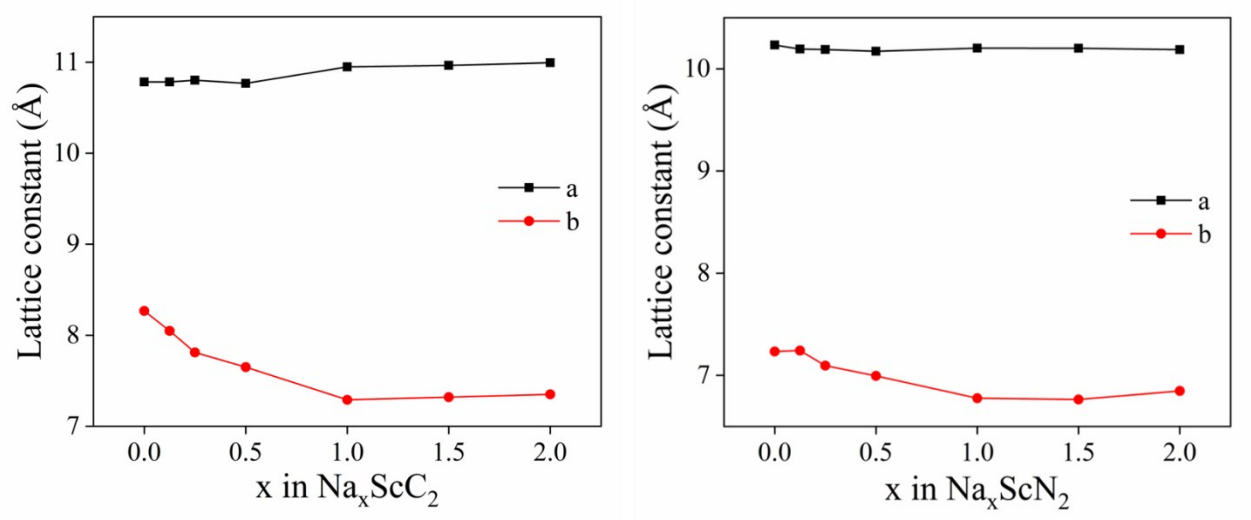

Figure S7. The in-plane lattice constants of Na_xScC_2 and Na_xScN_2 with different concentration of Na ions adsorption.

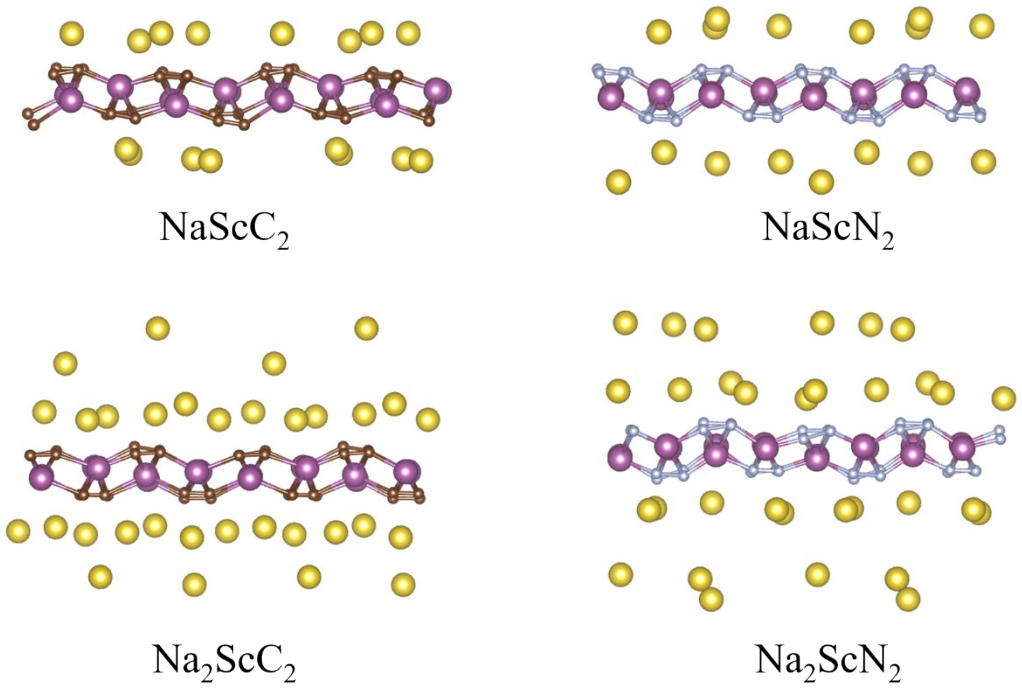

Figure S8. The configurational snapshots of $NaScC_2$, Na_2ScC_2, $NaScN_2$ and Na_2ScN_2 at 800 K in the end of 10 ps AIMD simulations.

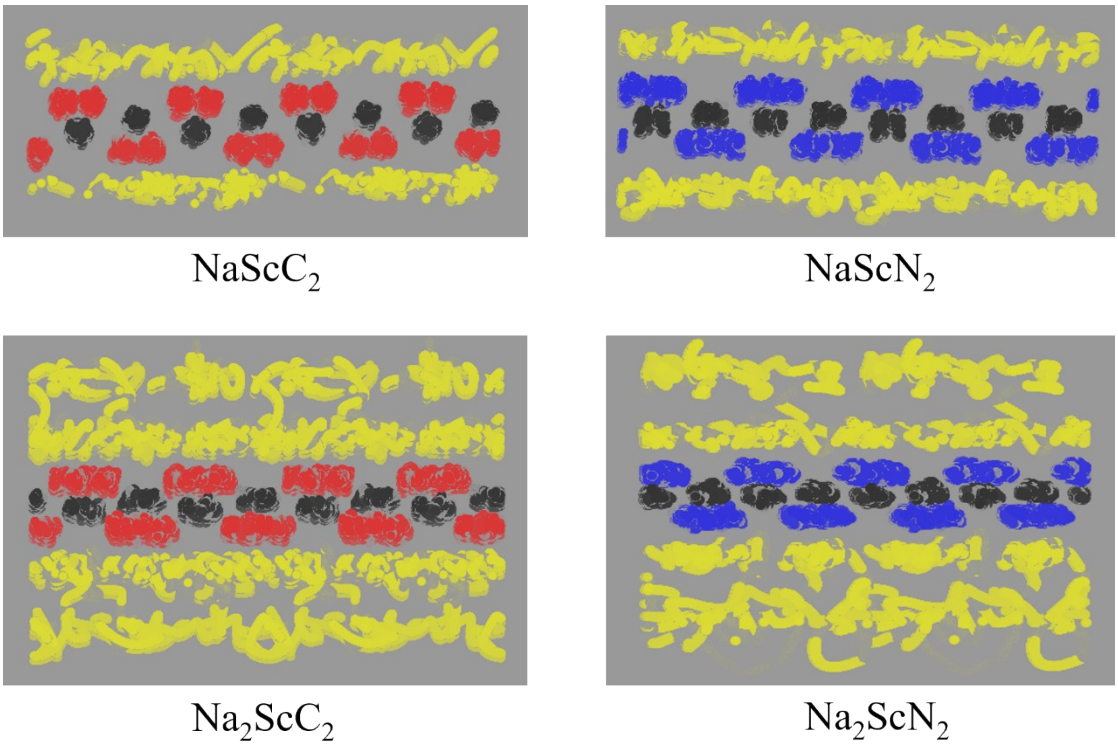

Figure S9. The atomic trajectories of $NaScC_2$, Na_2ScC_2, $NaScN_2$ and Na_2ScN_2 monolayers with the accumulation of the final 4000 AIMD simulation steps at 800 K. The black dots represent Sc atoms, the red dots represent C atoms, the blue dots represent N atoms, and the yellow dots represent Na atoms.

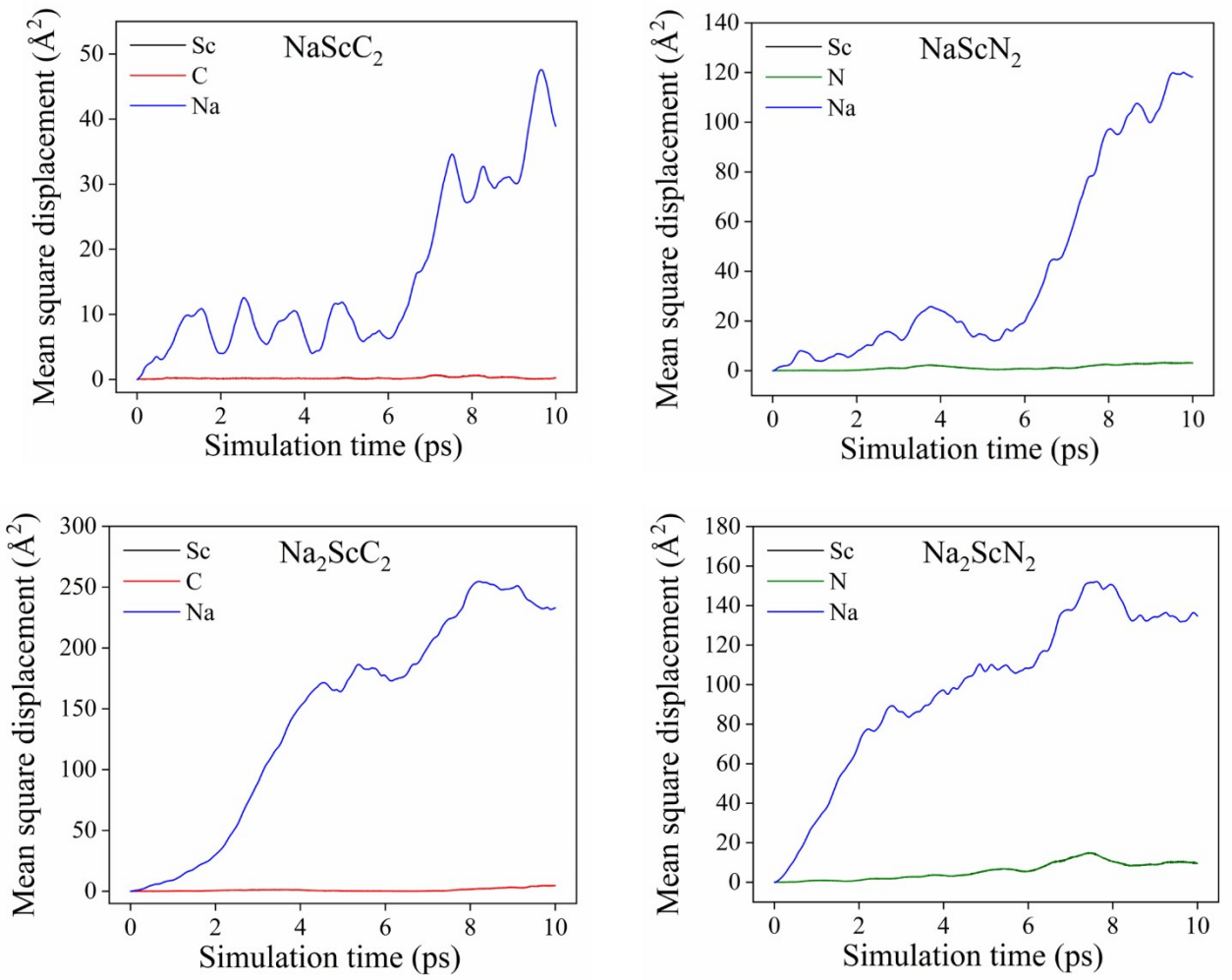

Figure S10. The total mean square displacements (MSD) of all atoms in $NaScC_2$, Na_2ScC_2, $NaScN_2$ and Na_2ScN_2 monolayers at 800 K. The AIMD simulations prove the thermodynamic stability of both o-ScC_2 and o-ScN_2 monolayers with relatively high concentration Na ion adsorption.