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

Supporting Information

Ab initio prediction of two-dimensional Si3C enabling high specific capacity as anode material in Li/Na/K-ion batteries

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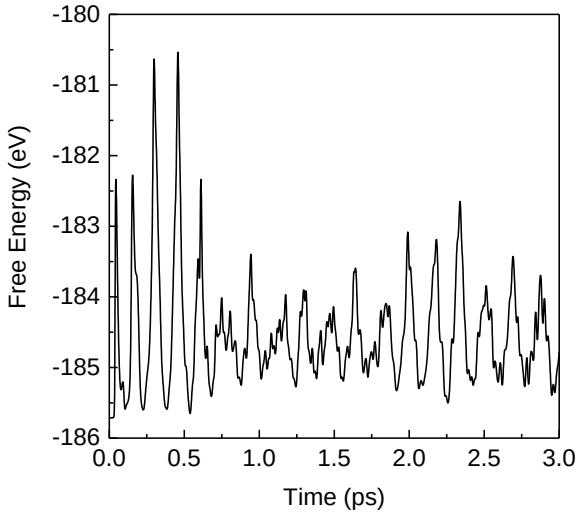
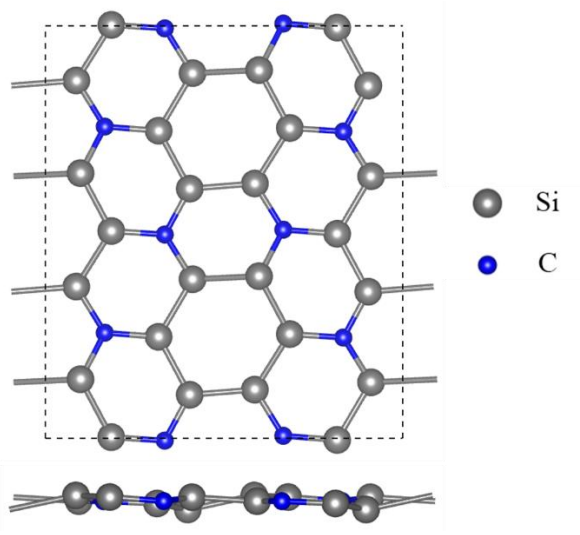


(a)



(b)

Figure S1. (a) Evolution of free energy of Si_3C monolayer during the AIMD simulation. (b) Snapshot of Si_3C monolayer from top and side views at 3ps.

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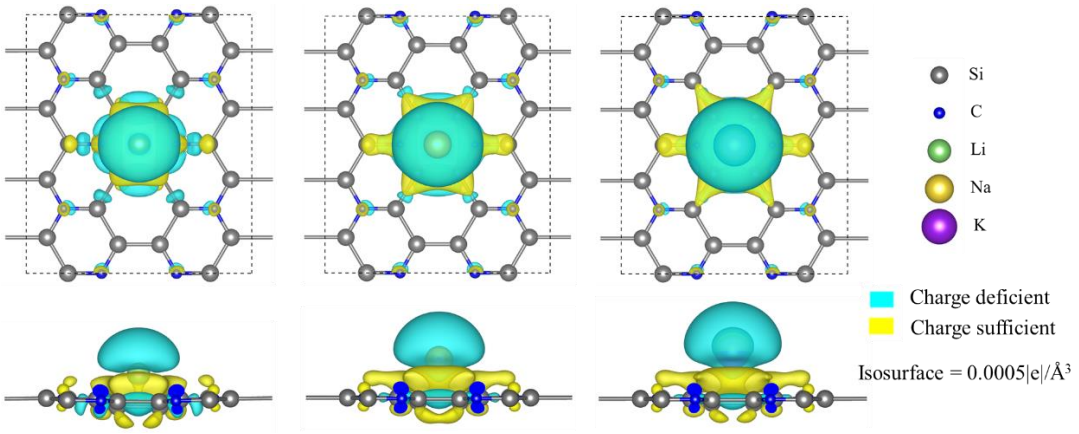
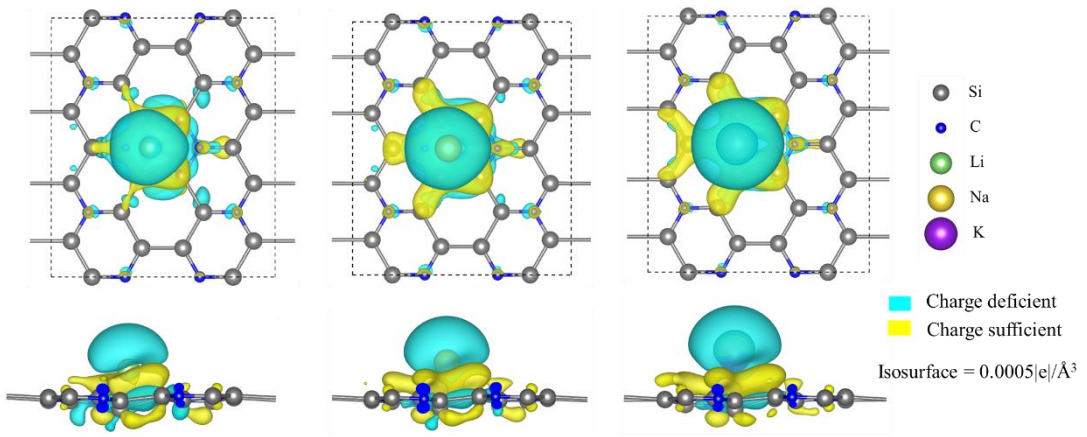


(a) (b) (c)

Figure S2. Optimized structures and charge difference plots of (a) Li, (b) Na and (c) K atoms adsorbed on H_2 site of Si_3C monolayer. The blue and yellow areas represent the charge deficient area and sufficient area, respectively.



(a) (b) (c)

Figure S3. Optimized structures and charge difference plots of (a) Li, (b) Na and (c) K atoms adsorbed on T_1, T_2 and B_2 sites of Si_3C monolayer. The blue and yellow areas represent the charge deficient area and sufficient area, respectively.

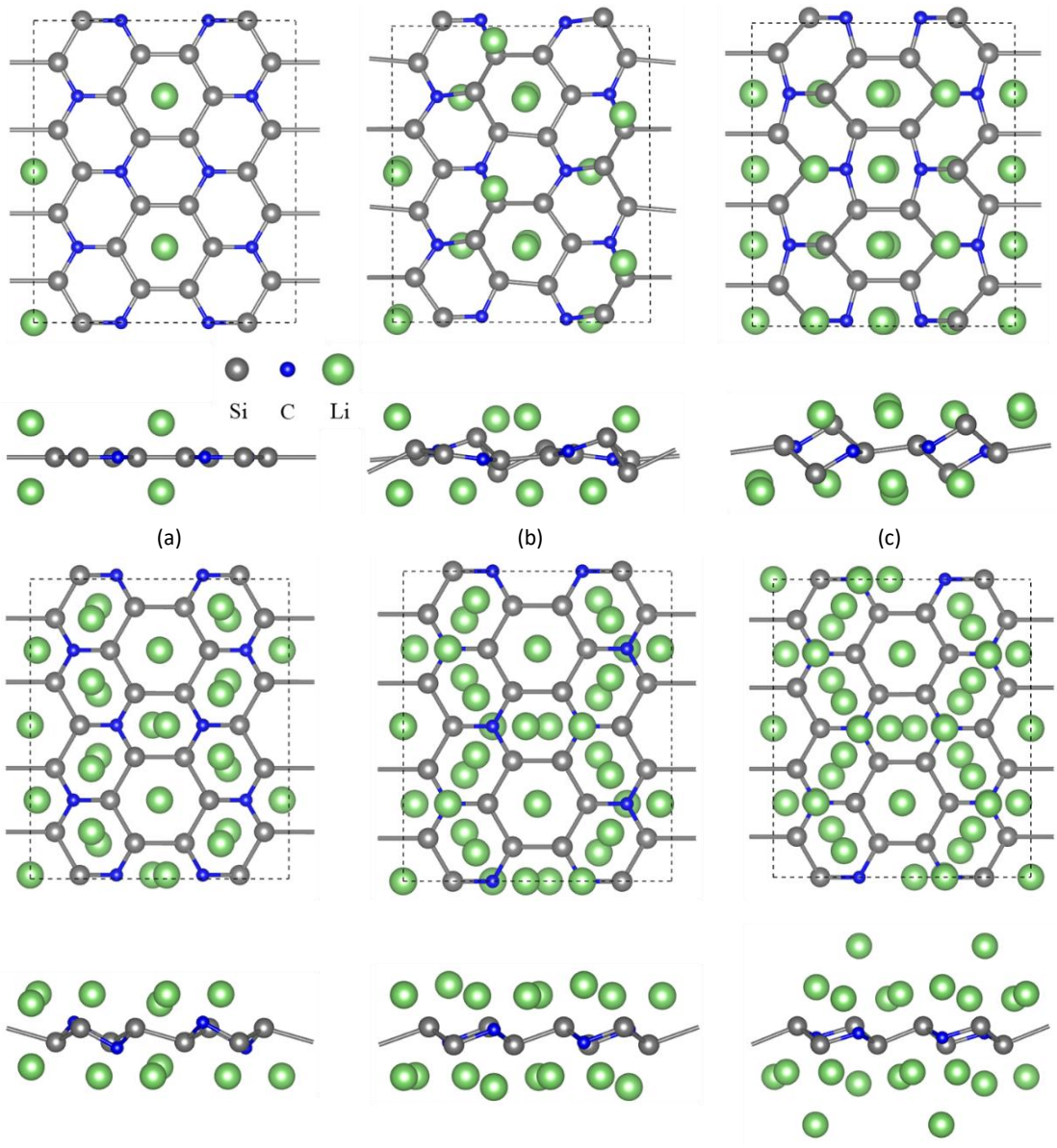


Fig. S4. Top and side views of the optimized structures for different Li concentrations. (a) $LiSi_3C$. (b) Li_2Si_3C. (c) Li_3Si_3C. (d) Li_4Si_3C. (e) Li_5Si_3C. (f) Li_6Si_3C.

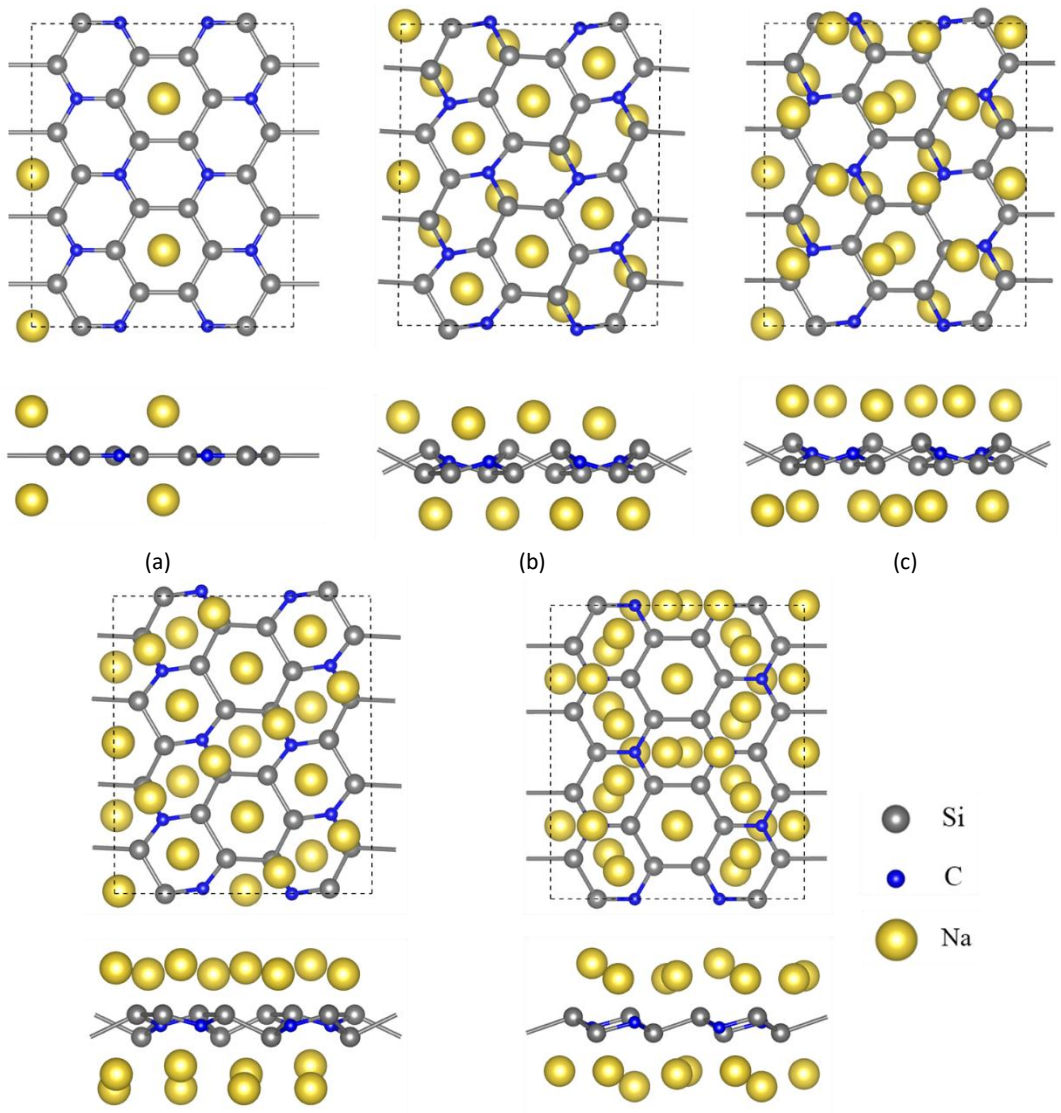


Fig. S5. Top and side views of the optimized structures for different Na concentrations. (a) $NaSi_3C$. (b) Na_2Si_3C. (c) Na_3Si_3C. (d) Na_4Si_3C. (e) Na_5Si_3C.

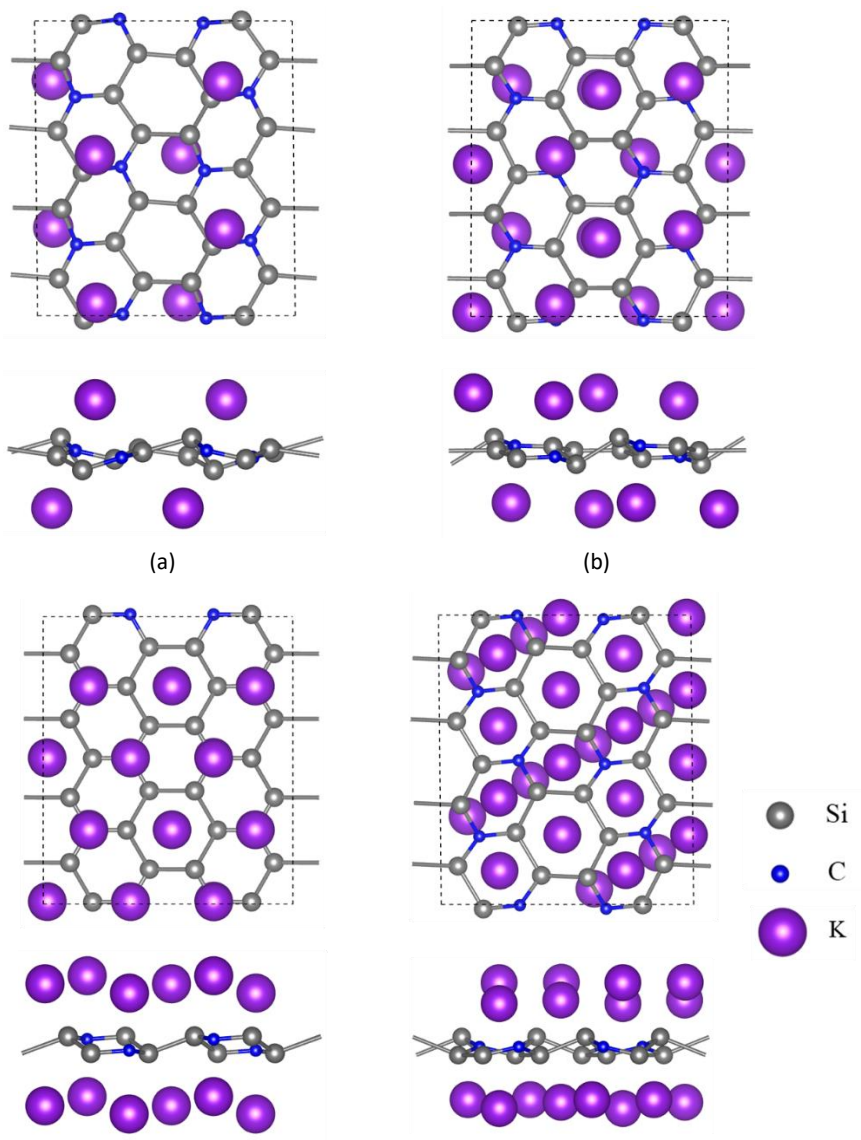


Fig. S6. Top and side views of the optimized structures for different K concentrations. (a) KSi_3C. (b) K_2Si_3C. (c) K_3Si_3C. (d) K_4Si_3C.

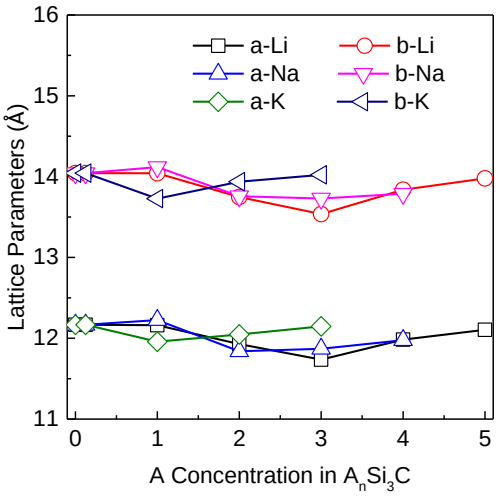


Fig. S7. Variation of lattice parameters of Si_3C monolayer for different Li/Na/K concentrations.