Electronic Supplementary Information (ESI)

A First-Principles Study on Si_{24} as an Anode Material for Rechargeable Batteries

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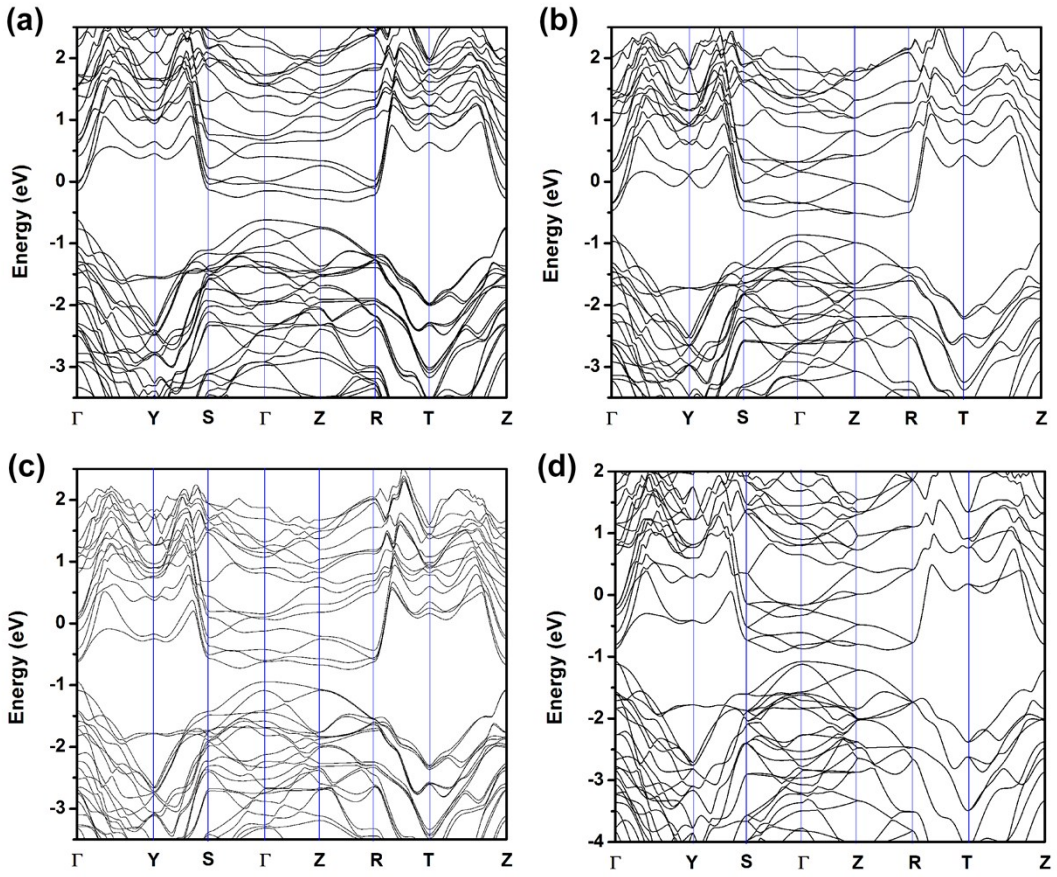

Fig. S1 Electronic band structures of (a) $LiSi_{24}$, (b)Li_2Si_{24}, (c)Li_3Si_{24} and (d)Li_4Si_{24}.

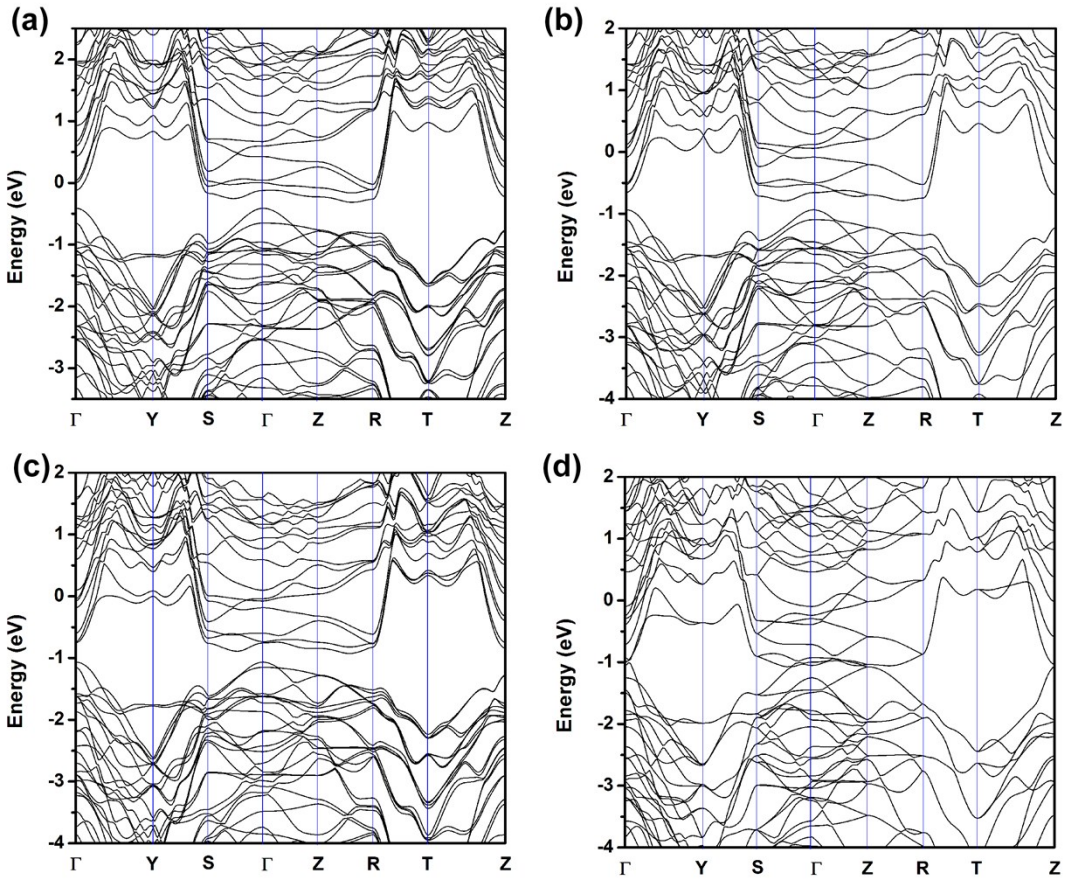

Fig. S2 Electronic band structures of (a) $NaSi_{24}$, (b)Na_2Si_{24}, (c)Na_3Si_{24} and (d)Na_4Si_{24}.

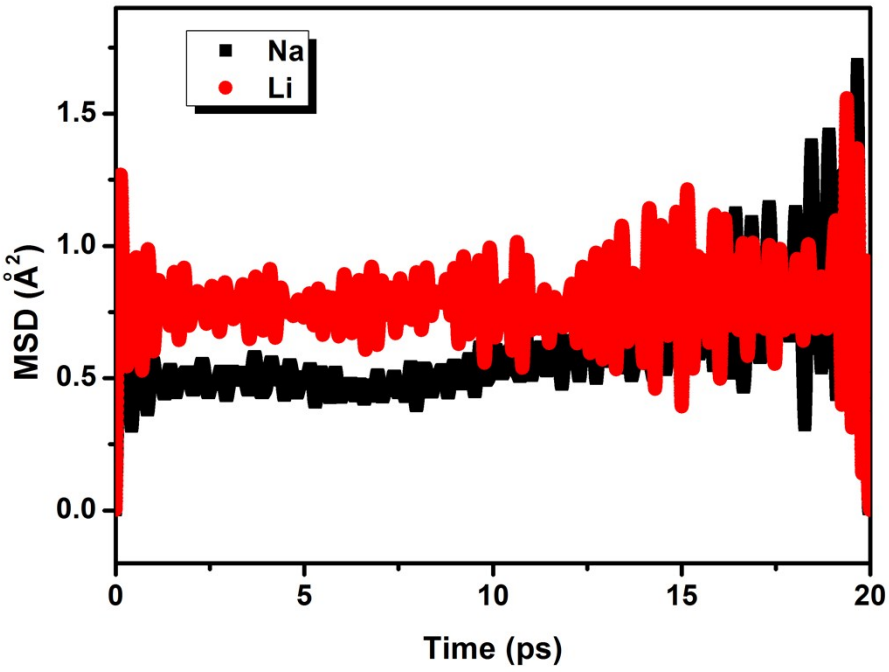

Fig. S3 MSD of Na/Li ions in Na_4Si_{24} and Li_4Si_{24} at temperature of 1500 K and 1000 K respectively.

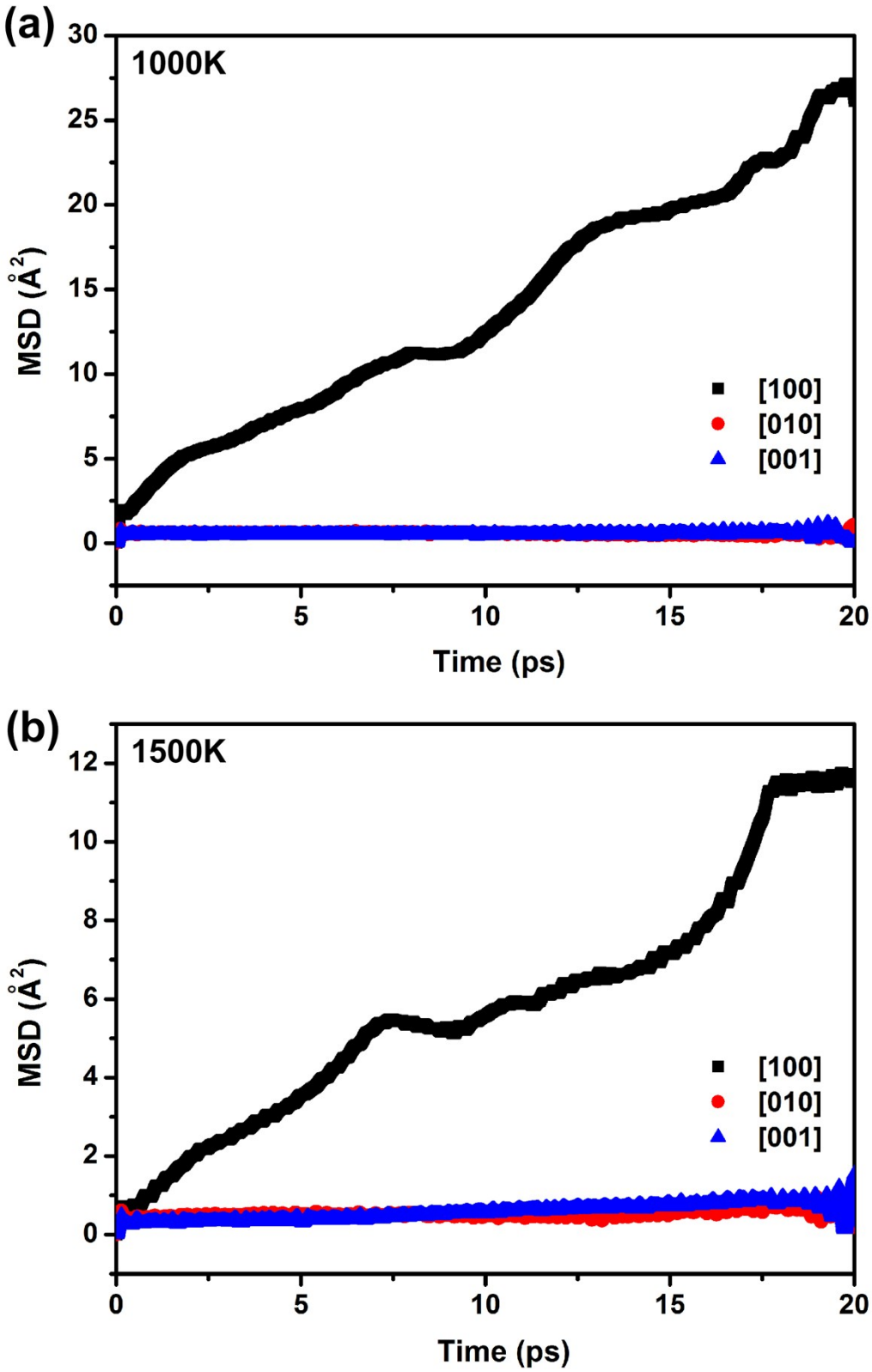

Fig. S4 Mean square displacement (MSD) of (a) Li^+ at 1000 K and (b) Na^+ at 1500 K in $Li_{2.66}Si_{24}$ and $Na_{2.66}Si_{24}$ along different lattice directions.

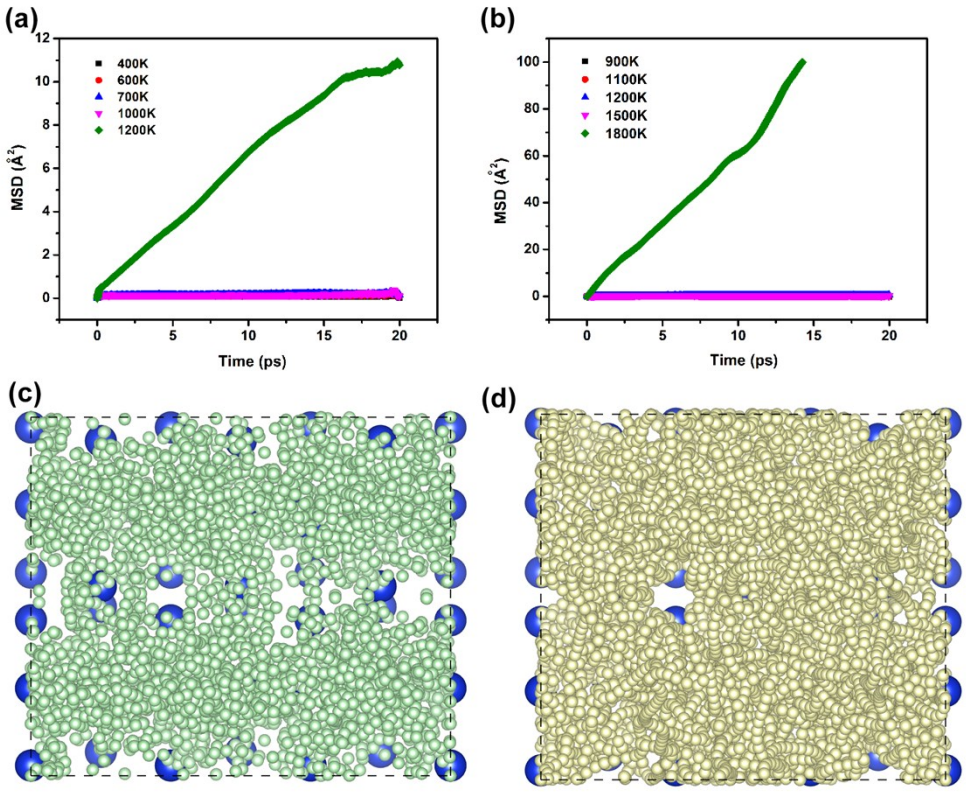

Fig. S5 Mean square displacement (MSD) of Li/Na ions in (a) $Li_{2.66}Si_{24}$ and (b) $Na_{2.66}Si_{24}$ at different temperature. Trajectories of (c) Li^+ at 1200 K in $Li_{2.66}Si_{24}$ and (d) Na^+ at 1800 K in $Na_{2.66}Si_{24}$.

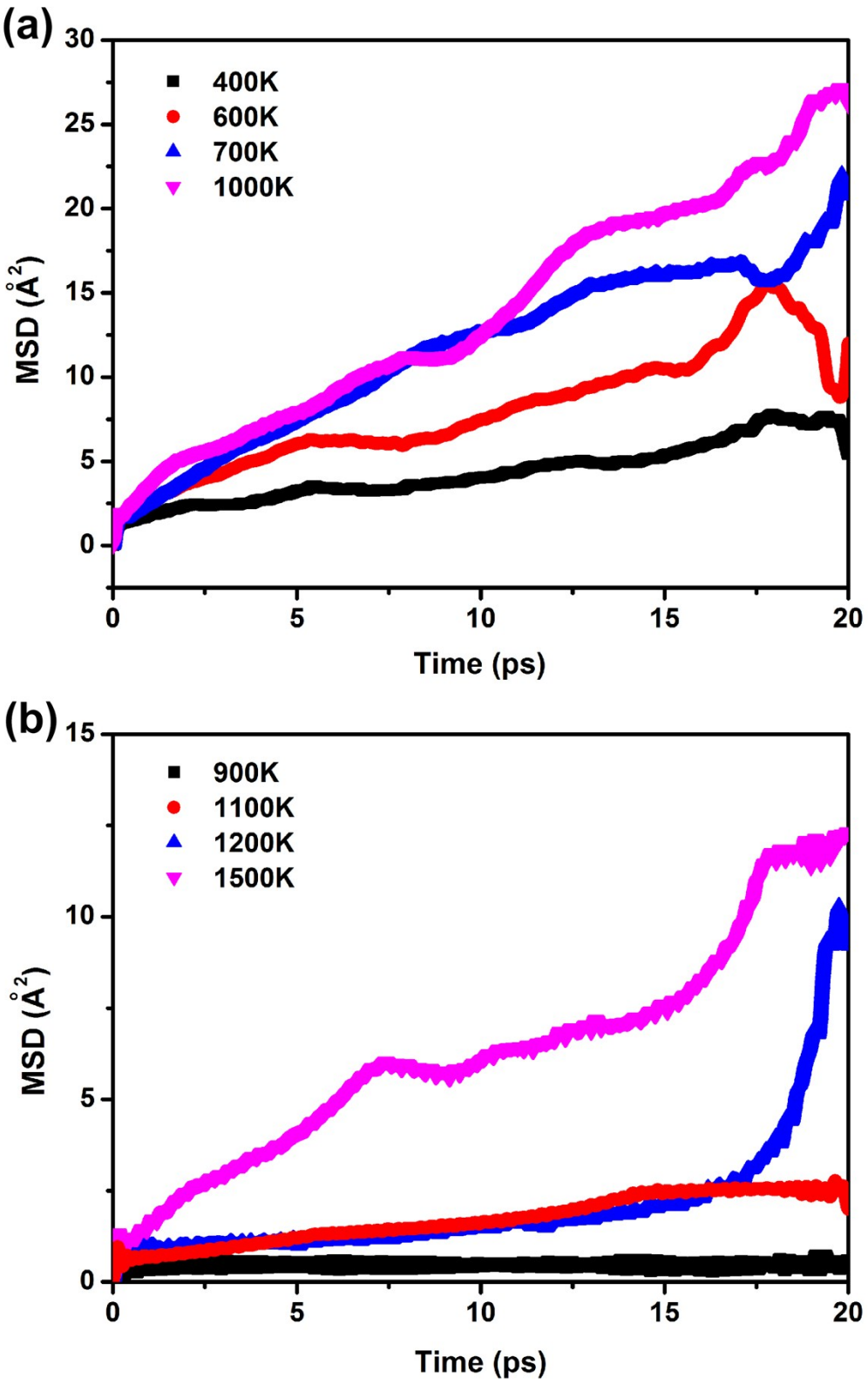

Fig. S6 Mean square displacement (MSD) of (a) Li^+ in $Li_{2.66}Si_{24}$ and (b) Na^+ in $Na_{2.66}Si_{24}$ at different temperatures.

Table S1 The comparison of volume per Si atom and theoretical capacity of Si and various Li-Si alloy.

Compound and crystal structure	Volume per Si atom ($Å^3$)	Theoretic capacity (mAh/g)
Si cubic	19.6	0
Li_4Si_{24} orthorhombic	22.0	159
LiSi tetragonal	31.4	954
$Li_{12}Si_7$ orthorhombic	43.5	1635
Li_2Si monoclinic	51.5	1900
$Li_{13}Si_4$ orthorhombic	67.3	3100
$Li_{15}Si_4$ tetragonal	76.4	3590
$Li_{22}Si_5$ cubic	82.4	4200