Supporting Information

Lithiation of SiO_2 in Li-ion Batteries: *in-situ* Transmission Electron Microscopy Experiments and Theoretical Studies

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Movie S1 The time evolution of a single nanowire upon two cycles of lithiation and delithiation.

Movie S2 Inhomogeneous growth of the SiO_2 thin layer upon two cycles of lithiation and delithiation.

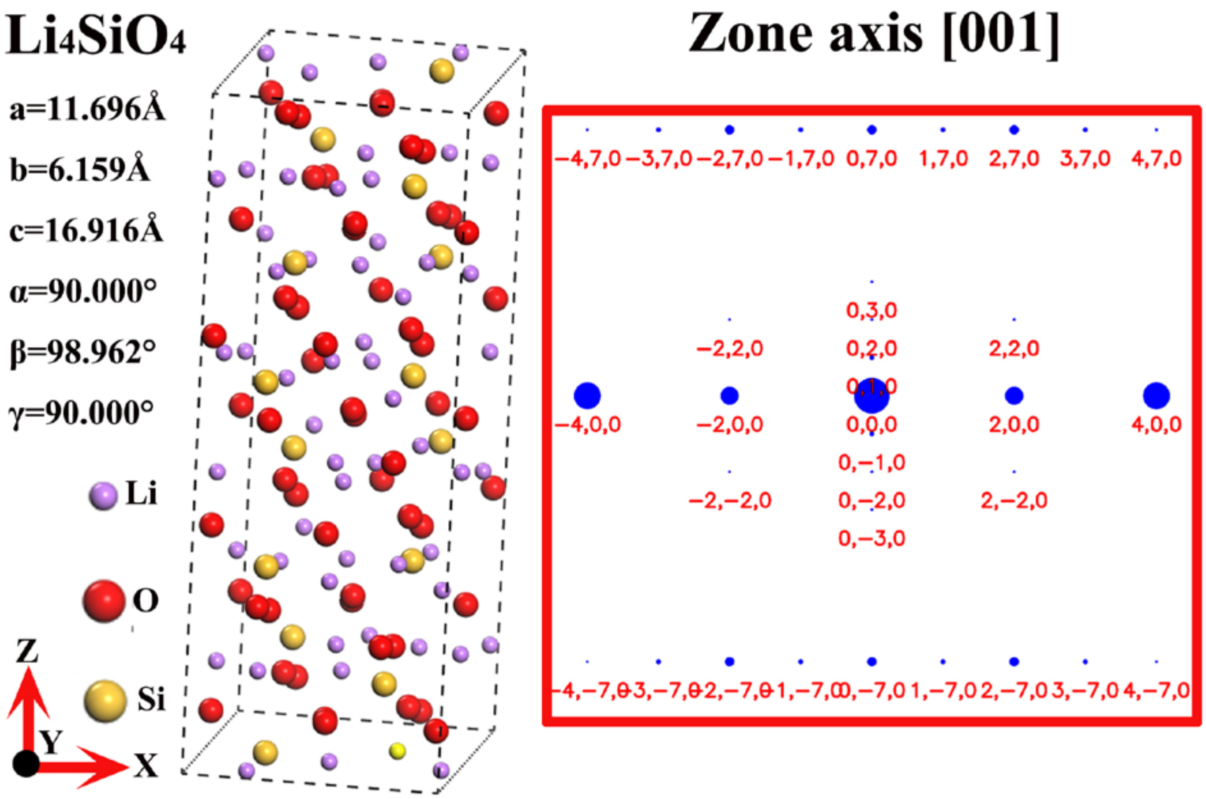

Figure S1 The crystal structure of Li_4SiO_4 and the simulated diffraction pattern.

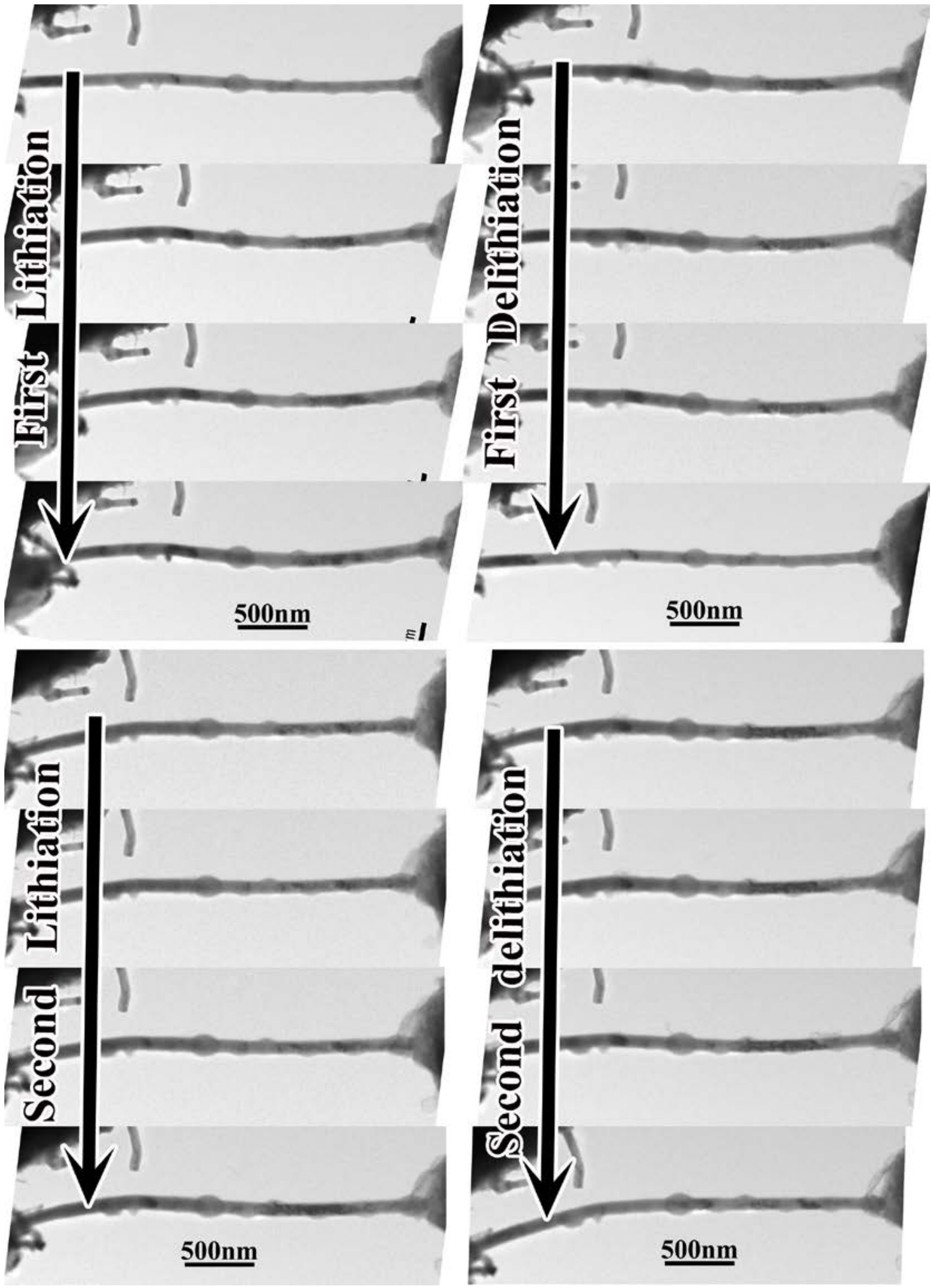

Figure S2 Non-uniform growth of the SiO_2 layer during the first two cycles of lithiation and delithiation.

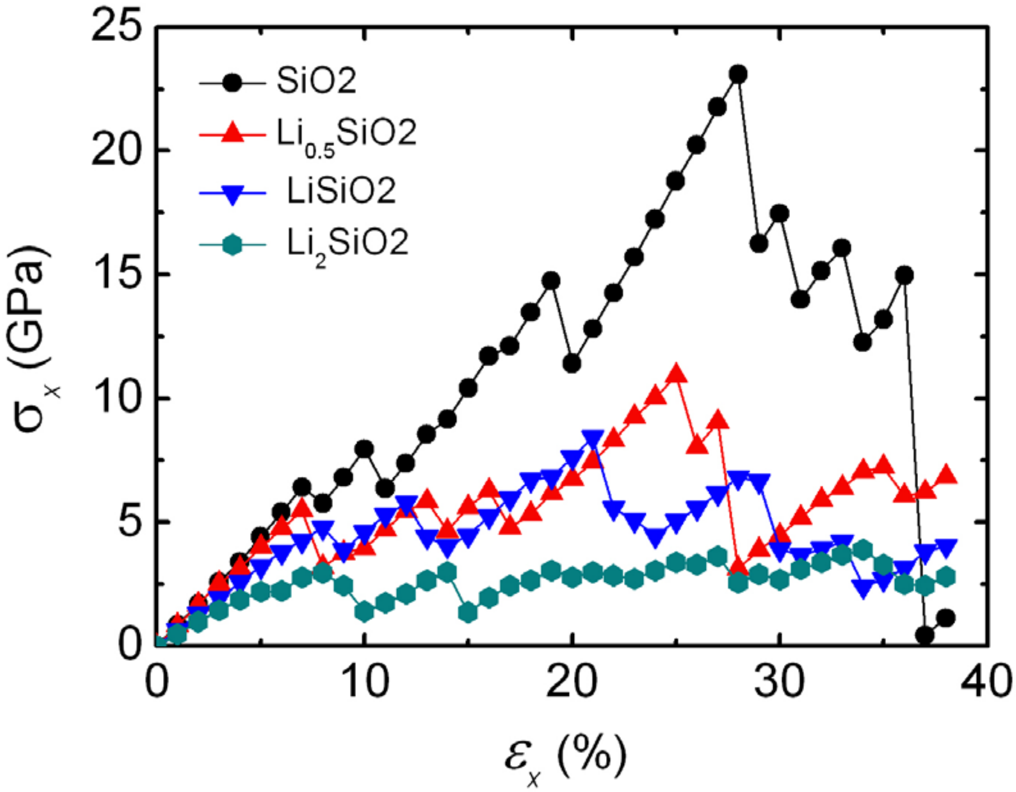

Figure S3 Stress-strain curves of a-Li_xSiO_2 under uniaxial deformation simulated using first-principles methods. An incremental strain is applied along the *x* direction of the Li_xSiO_2 supercell, and the responsive stress is recorded. The increase – drop in the stress is a feature of amorphous structure in small-scale modeling. Atoms in the lattice can release the stress by rearranging their positions. The solid symbols represent the calculation data. The lines connecting the data are guide for the eyes.

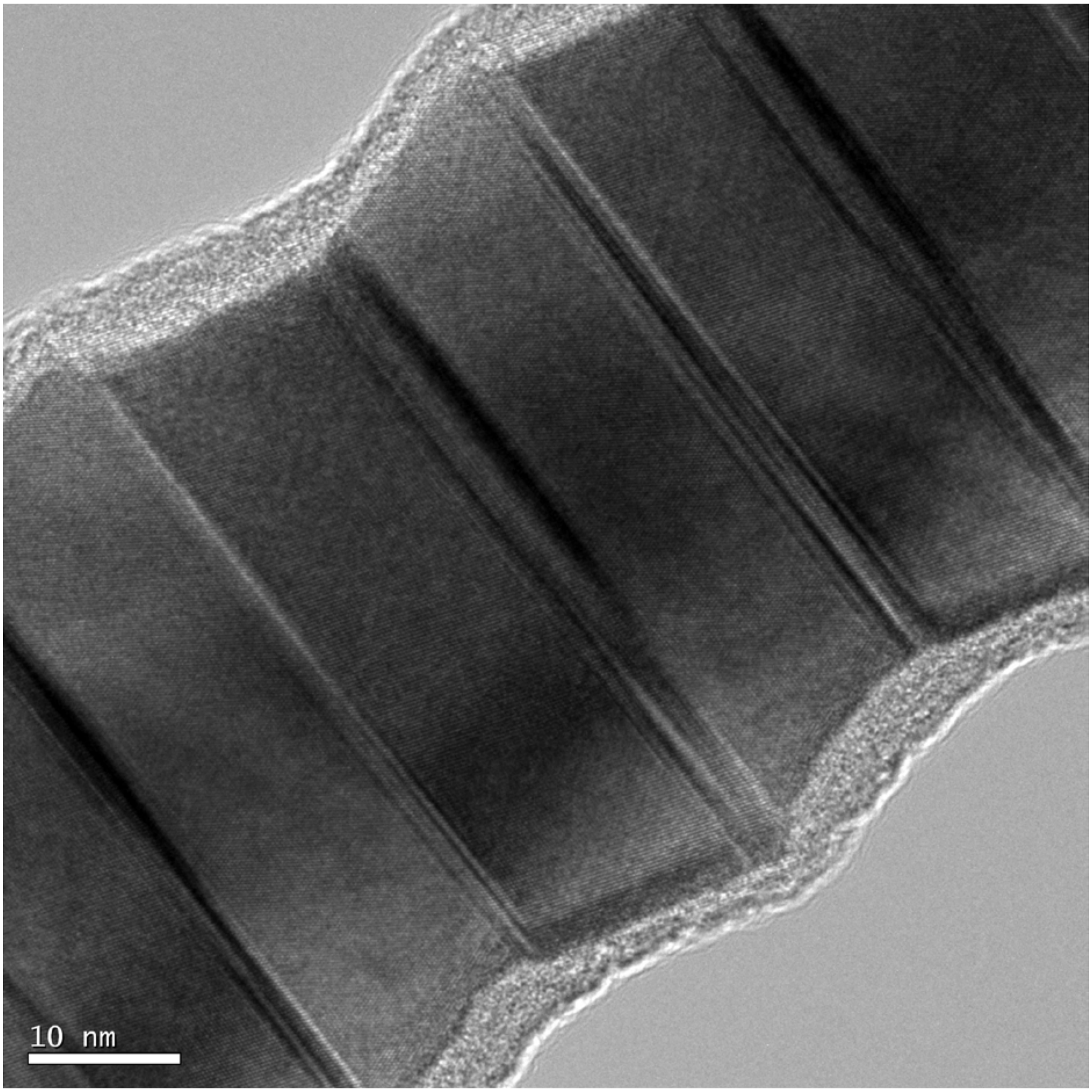

Figure S4 A high-resolution image of a SiO_2@SiC nanowire with alternative convex and concave surfaces.

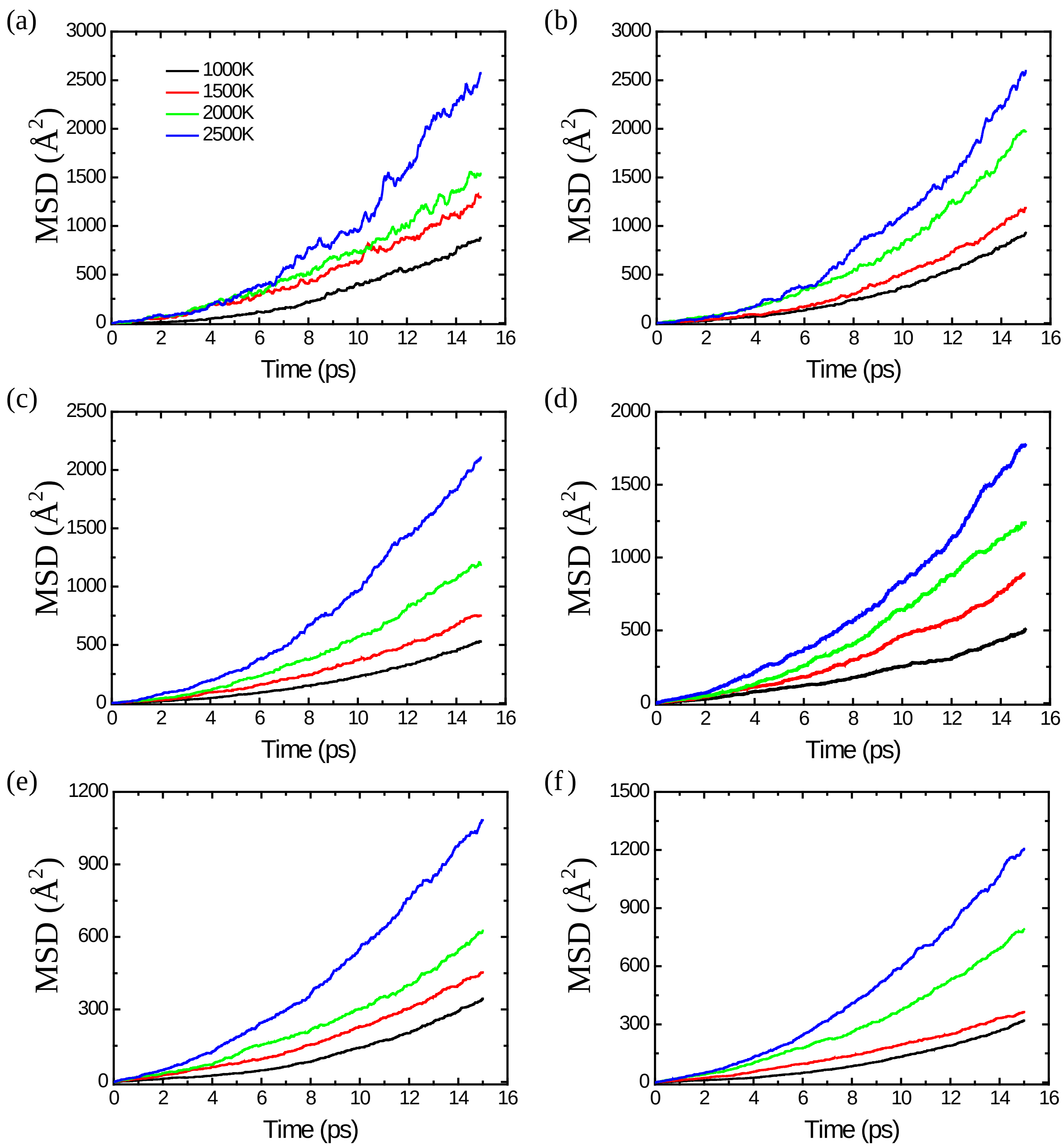

Figure S5 Mean square displacement of Li in (a) $Li_{0.125}SiO_2$, (b) $Li_{0.25}SiO_2$, (c) $Li_{0.5}SiO_2$, (d) $LiSiO_2$, (e) $Li_{1.5}SiO_2$, and (f) Li_2SiO_2. The black, red, green, and blue lines represent the calculation data at 1000, 1500, 2000, and 2500 K, respectively.

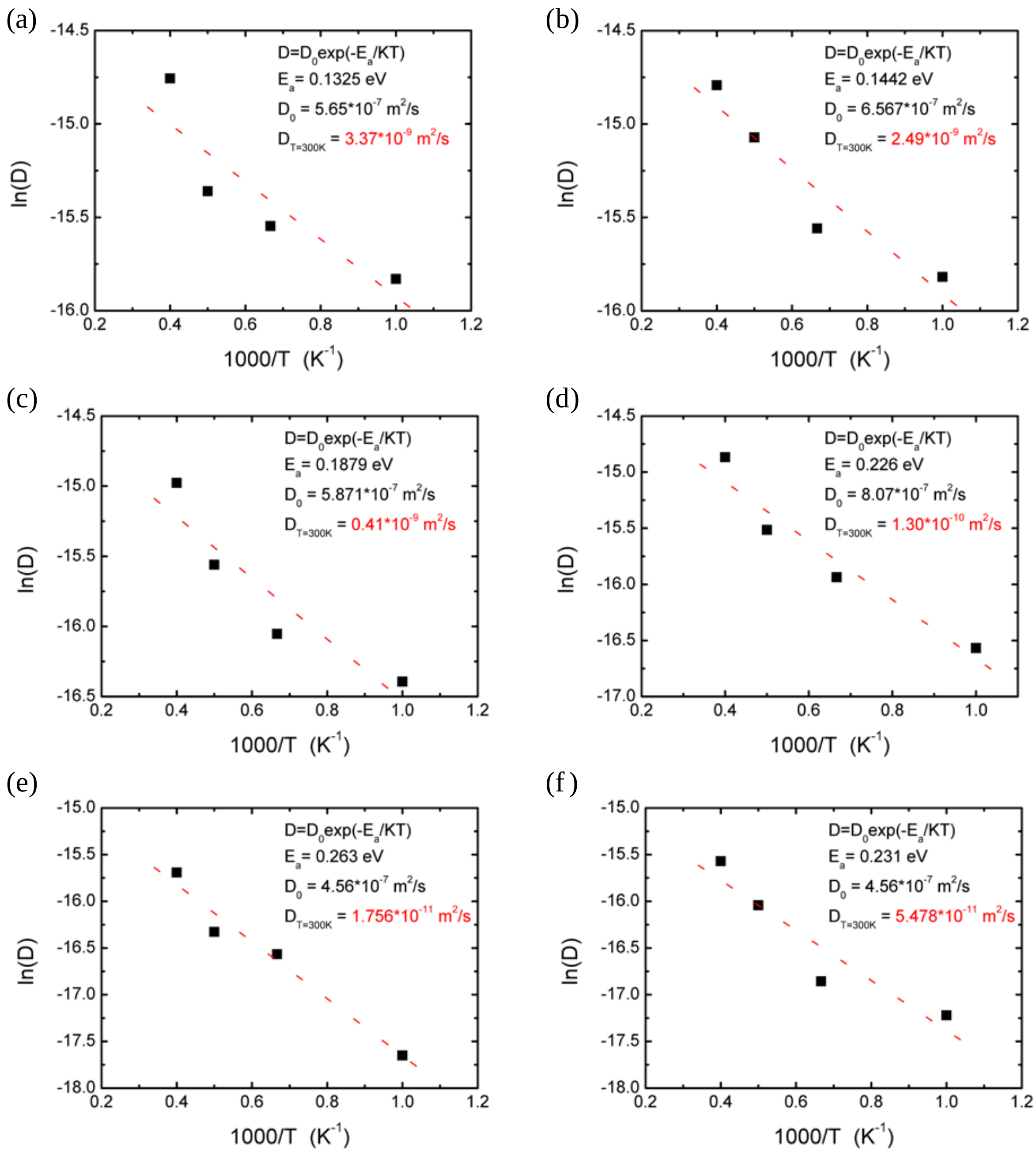

Figure S6 Derived diffusivity of Li at T=300 K in (a) $Li_{0.125}SiO_2$, (b) $Li_{0.25}SiO_2$, (c) $Li_{0.5}SiO_2$, (d) $LiSiO_2$, (e) $Li_{1.5}SiO_2$, and (f) Li_2SiO_2. The diffusivity was obtained by fitting the mean square displacement using $D = D_0 \exp(-E_a / kT)$.

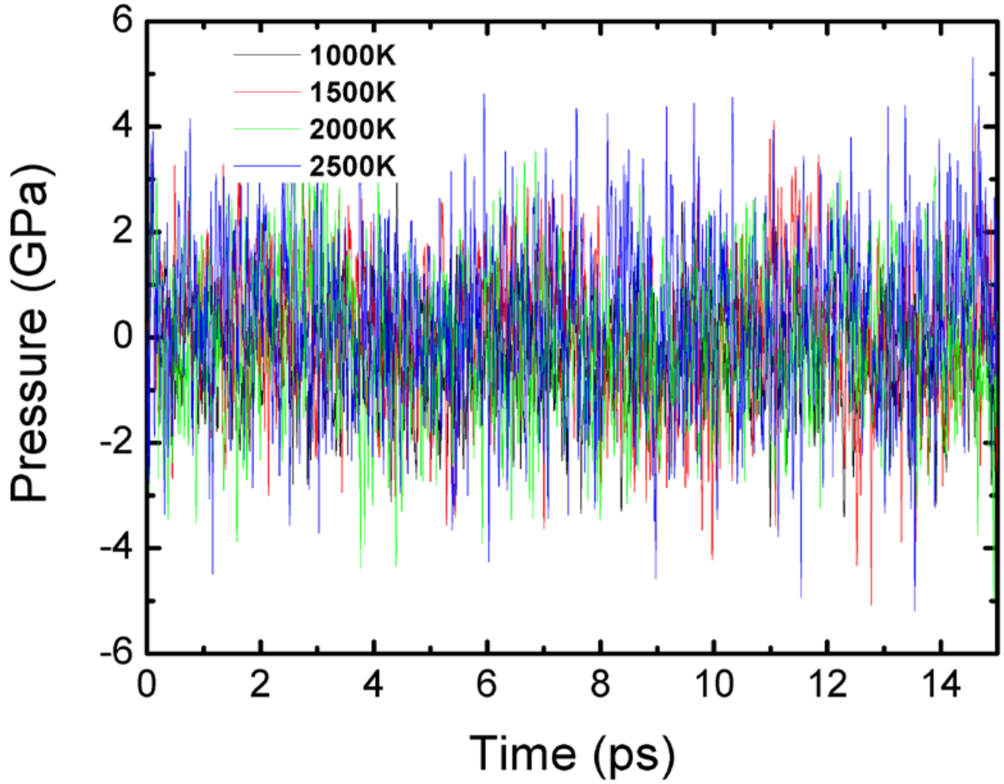

Figure S7 Pressure fluctuations in the supercell of $Li_{0.5}SiO_2$ at various temperatures. The average values of pressure are around zero during the MD simulations.