

Supplementary Information

for

**Unraveling the performance enhancement mechanism of Ti doping for Li₄SiO₄-
based solar energy storage: A combined experimental, kinetic, and DFT study**

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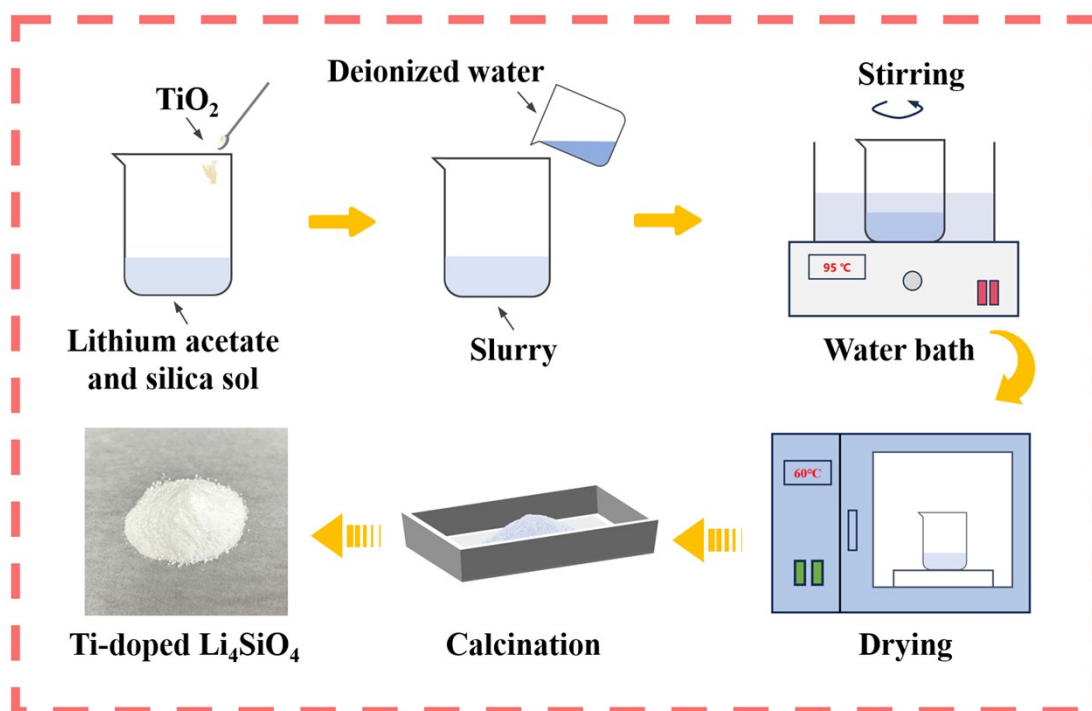


Fig. S1. Schematic presentation of synthesis of Ti-doped Li_4SiO_4

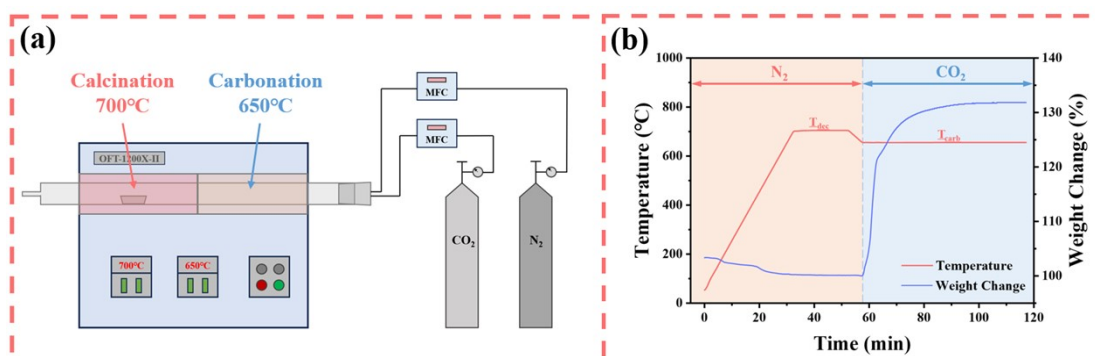


Fig. S2. Schematic of (a) experimental system based on dual fixed bed reactor; (b)

kinetic experiments for carbonation

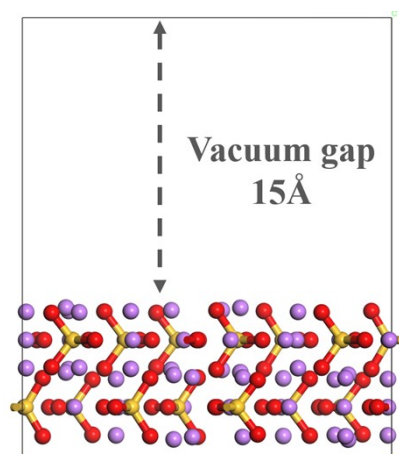


Fig. S3. Li_4SiO_4 (0 1 0) surface model (front view)

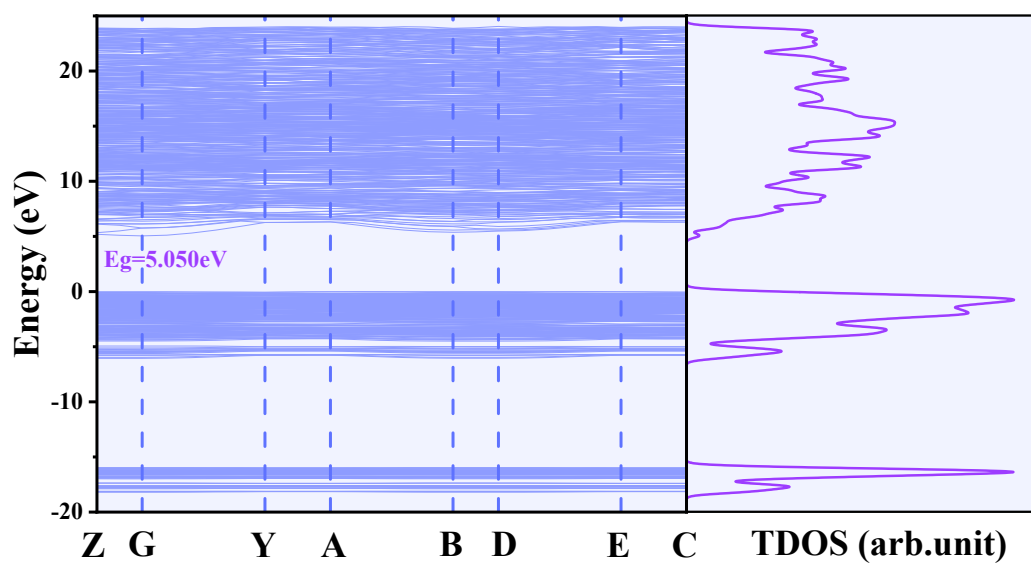


Fig. S4. The calculated electronic band structures and total density of states (TDOS)

values of pure Li_4SiO_4 crystal

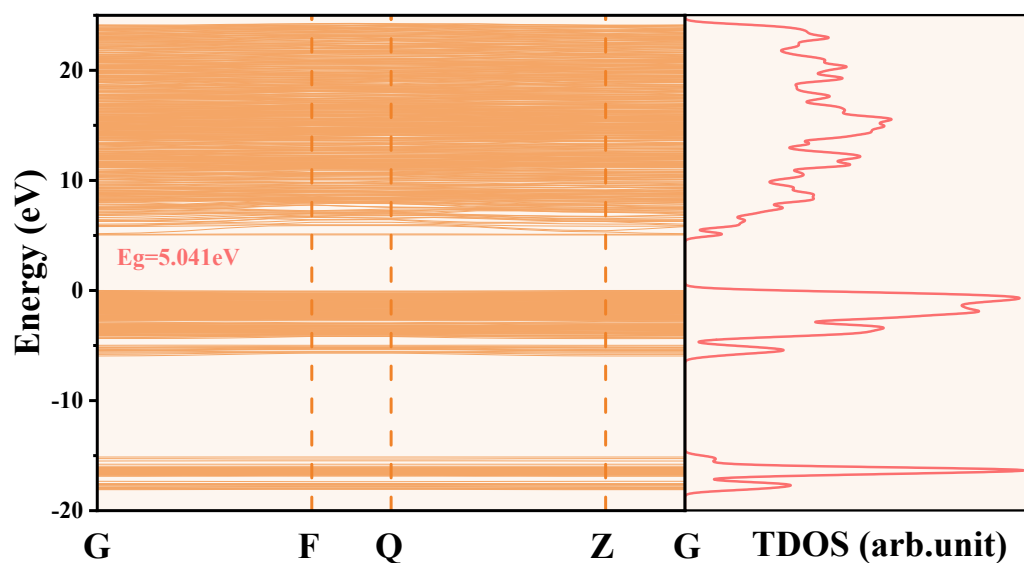


Fig. S5. The calculated electronic band structures and total density of states (TDOS)

values of Ti-doped Li_4SiO_4 crystal

Table S1

Kinetic parameters obtained from the isotherms of Li_4SiO_4 fitted to double-exponential model.

Sample	Temperature ($^{\circ}\text{C}$)	k_1 (s^{-1})	k_2 (s^{-1})	A	B	C	R^2
LA-0Ti	550	4.42×10^{-1}	1.73×10^{-2}	-5.06	-7.20	112.32	0.999
	600	9.18×10^{-1}	1.94×10^{-2}	-10.18	-10.87	118.49	0.999
	650	1.00×10	4.10×10^{-2}	-24.75	-17.17	133.52	0.999
LA-5Ti	550	3.86×10^{-1}	2.47×10^{-2}	-7.64	-8.15	116.05	0.998
	600	5.11×10^{-1}	2.23×10^{-2}	-10.50	-14.09	124.55	0.999
	650	7.45×10^{-1}	1.05×10^{-1}	-17.51	-14.42	131.80	0.999

Table S2

Kinetic parameters obtained from the isotherms of Li_4SiO_4 fitted to Jander model.

Sample	Temperature (°C)	k	R ²
LA-0Ti	550	1.35×10^{-4}	0.983
	600	3.72×10^{-4}	0.974
	650	5.47×10^{-3}	0.970
LA-5Ti	550	3.16×10^{-4}	0.980
	600	8.86×10^{-4}	0.994
	650	1.00×10^{-2}	0.985

Table S3

Kinetic parameters obtained from the isotherms of Li_4SiO_4 fitted to a Avrami-Erofeev model.

Sample	Temperature (°C)	Chemical-controlled stage			Diffusion-controlled stage		
		n	k ₁	R ²	n	k ₂	R ²
LA-0Ti	550	1.48	6.38×10^{-3}	0.983	0.61	1.73×10^{-3}	0.919
	600	1.64	4.01×10^{-3}	0.974	0.62	1.63×10^{-3}	0.888
	650	1.79	2.16×10^{-3}	0.970	0.70	1.53×10^{-3}	0.975
LA-5Ti	550	1.87	7.76×10^{-3}	0.980	0.59	2.00×10^{-3}	0.919
	600	1.79	4.65×10^{-3}	0.994	0.63	1.69×10^{-3}	0.897
	650	1.79	3.00×10^{-3}	0.985	0.86	2.91×10^{-3}	0.983