Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Material for

Facet-Dependent Lithium Intercalation into Si Crystal: Si(100) vs. Si(111)

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Table S1. Binding energies (E_b) of Li on the T4 and T4′ sites of Si(100) and diffusion barriers (E_d) of Li for pathways connecting the T4 and T4′ sites. N_{layer}, d_{vacuum}, k-point mesh, and E_{cut} represent the number of Si layers in the slab, the vacuum spacing between the slabs, the subdivisions of the (4 × 2) surface Brillouin zone, and the plane-wave cut-off energy, respectively. ΔE_b represents the difference between the T4 and T4′ binding energies. The energy units are given in eV.

N_{layer}	d_{vacuum} (Å)	k-point mesh	E_{cut}	E_b		ΔE_b	E_d	
				T4	T4′		T4 → T4′	T4′ → T4
14	12.2	2×4×1	245.3	2.383	2.262	0.121	0.364	0.243
18	12.2	2×4×1	245.3	2.377	2.257	0.120	0.363	0.243
14	14.9	2×4×1	245.3	2.380	2.256	0.124	0.364	0.240
14	12.2	3×6×1	245.3	2.465	2.349	0.116	0.367	0.251
14	12.2	2×4×1	306.6	2.393	2.268	0.125	0.360	0.236

Table S2. Binding energies (E_b) of Li at the surface and subsurface sites of Si(100) and Si(111). $d_{Li–Si}$ denotes the average distance between the Li atom and its nearest Si atoms.

Si(100)			Si(111)		
Sites	E_b (eV)	$d_{Li–Si}$ (Å)	Sites	E_b (eV)	$d_{Li–Si}$ (Å)
T4 (T4′)	2.38 (2.26)	2.63 (2.77)	H3 (H3′)	2.42 (2.02)	2.55 (2.64)
S1 (S1′)	1.85 (1.82)	2.43 (2.50)	S1 (S1′)	1.77 (1.74)	2.44 (2.51)
S2	1.77	2.46	S2	1.75	2.46
S3	1.68	2.47	S3	1.46	2.46
S4	1.59	2.45	S4	1.46	2.47
S5	1.55	2.45	S5	1.30	2.45
bulk	1.28	2.45	bulk	1.28	2.45

Fig. S1. Surface geometries of (a) Si(100)-c(4 × 2) and (b) Si(100)-p(2 × 2). In (a) and (b), the T4 sites have different nearest neighbors: two up Si atoms in c(4 × 2) and one up Si and one down Si atoms in p(2 × 2).