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*Supplementary Material for*

# Lithium Intercalation Behaviors in Ge and Sn Crystalline Surfaces

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**Table S1**. Binding energies ($E_b$) of Li on the T4 and T4´ sites of Ge(100) and diffusion barriers ($E_d$) of Li for pathways connecting the two 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. $\Delta E_b$ 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 | $E_{cut}$ | $E_b$ | | $\Delta E_b$ | $E_d$ | |
|---|---|---|---|---|---|---|---|---|
| | | | | T4 | T4′ | | T4 → T4′ | T4′ → T4 |
| 14 | 11.5 | 2 x 4 x 1 | 173.8 | 2.201 | 2.255 | 0.054 | 0.252 | 0.307 |
| 18 | 11.5 | 2 x 4 x 1 | 173.8 | 2.177 | 2.229 | 0.052 | 0.251 | 0.303 |
| 14 | 14.4 | 2 x 4 x 1 | 173.8 | 2.179 | 2.233 | 0.054 | 0.250 | 0.304 |
| 14 | 11.5 | 3 x 6 x 1 | 173.8 | 2.258 | 2.312 | 0.054 | 0.256 | 0.310 |
| 14 | 11.5 | 2 x 4 x 1 | 217.3 | 2.186 | 2.240 | 0.054 | 0.251 | 0.306 |

**Table S2**. Binding energies ($E_b$) of Li on the T4 and T4´ sites of Sn(100) and diffusion barriers ($E_d$) of Li for pathways connecting the two sites.

| $N_{layer}$ | $d_{vacuum}$ (Å) | k-point mesh | $E_{cut}$ | $E_b$ | | $\Delta E_b$ | $E_d$ | |
|---|---|---|---|---|---|---|---|---|
| | | | | T4 | T4′ | | T4 → T4′ | T4′ → T4 |
| 14 | 13.3 | 2 x 4 x 1 | 140.0 | 2.048 | 2.121 | 0.072 | 0.258 | 0.309 |
| 18 | 13.3 | 2 x 4 x 1 | 140.0 | 2.047 | 2.119 | 0.071 | 0.258 | 0.330 |
| 14 | 16.6 | 2 x 4 x 1 | 140.0 | 2.058 | 2.130 | 0.072 | 0.258 | 0.330 |
| 14 | 13.3 | 3 x 6 x 1 | 140.0 | 2.107 | 2.169 | 0.062 | 0.254 | 0.315 |
| 14 | 13.3 | 2 x 4 x 1 | 175.0 | 2.061 | 2.133 | 0.071 | 0.259 | 0.330 |

**Fig. S1**. Cross sections of bulk Si, Ge, and Sn along the <100> and <111> directions. Crosses and triangles represent the tetrahedral and hexagonal sites, respectively, and a, b, b′, and c represent the distances between the adjacent tetrahedral (or hexagonal) sites along each direction. In Si, a, b, b′, and c are 1.37, 0.79, 2.37, and 1.58 Å, respectively. In Ge, a, b, b′, and c are 1.44, 0.83, 2.50, and 1.67 Å. respectively. In Sn, a, b, b′, and c are 1.66, 0.96, 2.88, and 1.92 Å. respectively.