

Supporting Information:

Theoretical Insights into 2D Siloxene as a Promising Anode Material for Lithium-Ion Batteries

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Table.S1. The working voltage (OCV), theoretical Li-ion storage capacity (SC), and the change in the lattice parameter (Δa , Δb) of siloxene monolayer during lithiation process.

System	OCV (V)	SC(mAh/g)	Δa (%), Δb (%)
Li ₈ @siloxene	1.52	180.67	0.08, 0.03
Li ₁₆ @siloxene	1.05	361.34	0.13, 0.09
Li ₂₅ @siloxene	0.84	564.59	1.76, 1.45
Li ₃₄ @siloxene	0.28	767.84	2.56, 2.23
Li ₄₂ @siloxene	0.26	948.51	3.95, 3.29
Li ₅₀ @siloxene	0.06	1129.18	4.25, 3.85

Table.S2: The lattice parameters a , b , and angles of pristine siloxene, and Li₅₀@siloxene are presented, with the numbers in parentheses indicating the percentage of structural deformation.

Lattice parameters	a (Å)	b (Å)	α, β, γ
pristine siloxene	15.607	16.271	90.0, 89.989, 120.0
Li ₅₀ @siloxene	15.603 (4.25%)	16.204 (3.85%)	89.99, 89.982, 120.08