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Ab initio prediction of silicene and graphene heterostructure as an anode material for Li- and Na-ion batteries

Supporting Information

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Table S1. Binding energy and charge transfer for lithium and sodium adsorbed onto silicene and graphene

	Silicene/Li				Graphene/Li		
Site	A1	A2	A3	A4	B1	B2	B3
E_b(eV)	-0.87	-0.58	-0.58	-0.43	-0.02	+0.36	+0.08
$\Delta Q_{Li(\|e\|)}$	+0.88	+0.89	+0.89	+0.89	+0.91	+0.92	+0.92
	Silicene/Na				Graphene/Na		
Site	A1	A2	A3	A4	B1	B2	B3
E_b(eV)	-0.84	-0.63	-0.63	-0.51	+0.03	+0.16	+0.04
$\Delta Q_{Na(\|e\|)}$	+0.86	+0.88	+0.88	+0.88	+0.86	+0.84	+0.84

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Table S2. Binding energy, charge transfer and equilibrium interlayer spacing for lithium and sodium adsorbed on the outside surface of silicene in the Si/G heterostructure

	Li/Si/G					Na/Si/G				
Site	Si1	Si2	Si3	Si4	Si5	Si1	Si2	Si3	Si4	Si5
E_b(eV)	-1.03	-1.04	-1.03	-1.00	-1.04	-0.96	-0.98	-0.96	-0.93	-0.98
$\Delta Q_{Li/Na}(\lvert e\rvert)$	+0.87	+0.88	+0.87	+0.88	+0.88	+0.86	+0.86	+0.86	+0.86	+0.86
$D_{Si\text{-}G}$(Å)	3.53	3.52	3.53	3.55	3.52	3.52	3.52	3.52	3.53	3.52

Table S3 Binding energy, charge transfer and equilibrium interlayer spacing for lithium and sodium adsorbed between the silicene and graphene in the Si/G heterostructure

	Si/Li/G					Si/Na/G				
Site	Si1	Si2	Si3	Si4	Si5	Si1	Si2	Si3	Si4	Si5
E_b(eV)	-1.50	-1.55	-1.50	-1.51	-1.55	-1.27	-1.33	-1.27	-1.29	-1.33
$\Delta Q_{\underline{\quad Li}}(\lvert e\rvert)$	+0.86	+0.86	+0.86	+0.87	+0.86	+0.86	+0.86	+0.83	+0.84	+0.83
$D_{Si\text{-}G}$(Å)	3.70	3.67	3.70	3.70	3.67	4.05	4.01	4.05	4.04	4.01

Table S4 Binding energy, charge transfer and equilibrium interlayer spacing for lithium and sodium adsorbed on the outside surface of graphene in the Si/G heterostructure

Si/G/Li							
Site	G1	G2	G3	G4	G5	G6	G7
E_b(eV)	-0.19	-0.20	-0.19	-0.19	-0.20	-0.19	-0.19
$\Delta Q_{Li/Na}$(|e|)	+0.91	+0.91	+0.91	+0.91	+0.91	+0.91	+0.91
$D_{Si\text{-}G}$(Å)	3.69	3.69	3.69	3.69	3.68	3.69	3.69
Si/G/Na							
Site	G1	G2	G3	G4	G5	G6	G7
E_b(eV)	-0.12	-0.12	-0.12	-0.12	-0.12	-0.12	-0.12
$\Delta Q_{Li/Na}$(|e|)	+0.93	+0.93	+0.93	+0.93	+0.93	+0.93	+0.93
$D_{Si\text{-}G}$(Å)	3.68	3.68	3.68	3.68	3.68	3.68	3.68

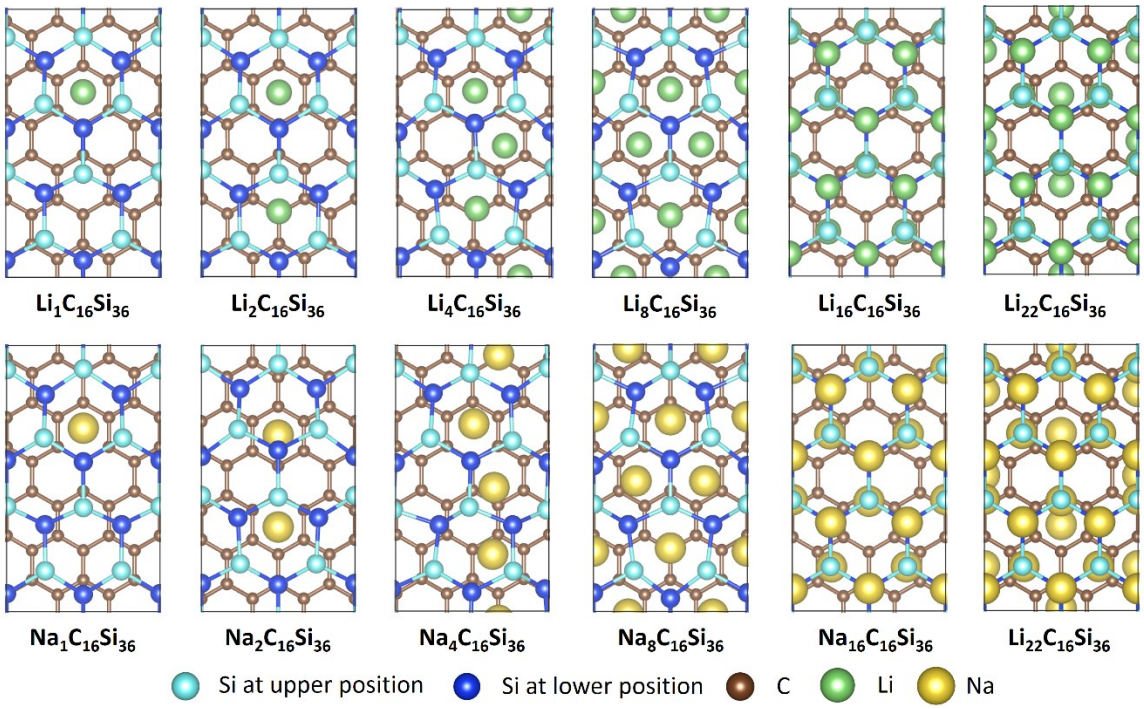

Fig. S1. The optimized structure of $Li/Na_xSi_{16}C_{36}$ with different lithium/sodium concentrations.

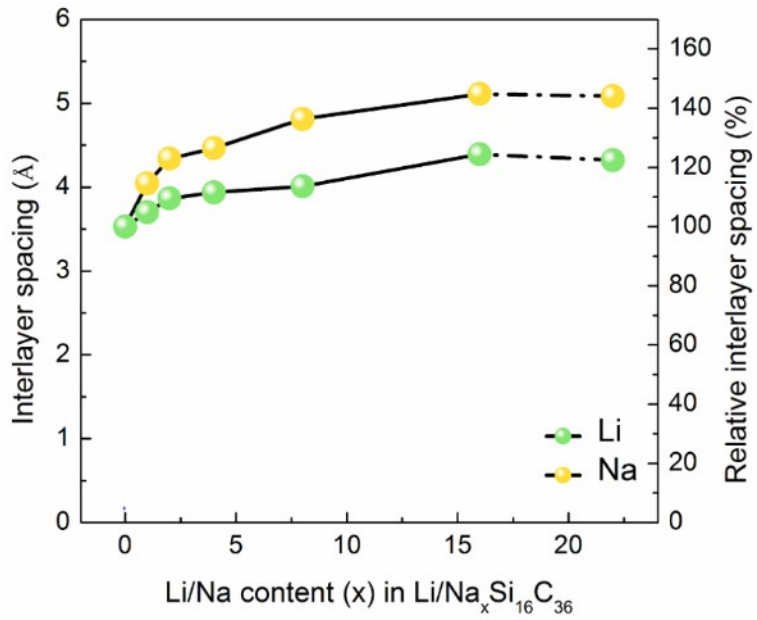

Fig. S2. Interlayer spacing expansion along with the intercalation process