Supporting Information

Defective Graphene/SiGe heterostructure as anodes of Li-ion Batteries: A first-principles calculations

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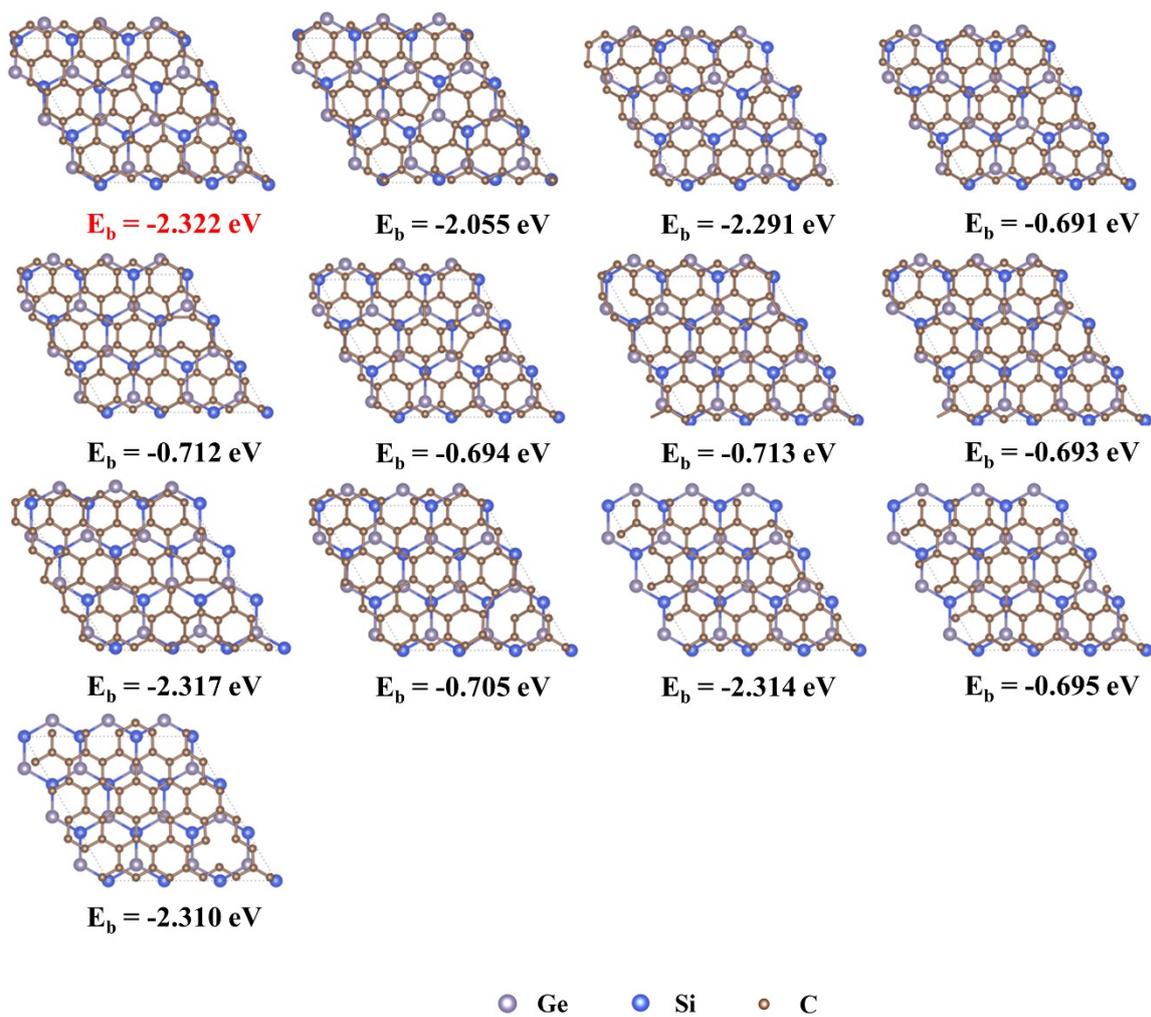
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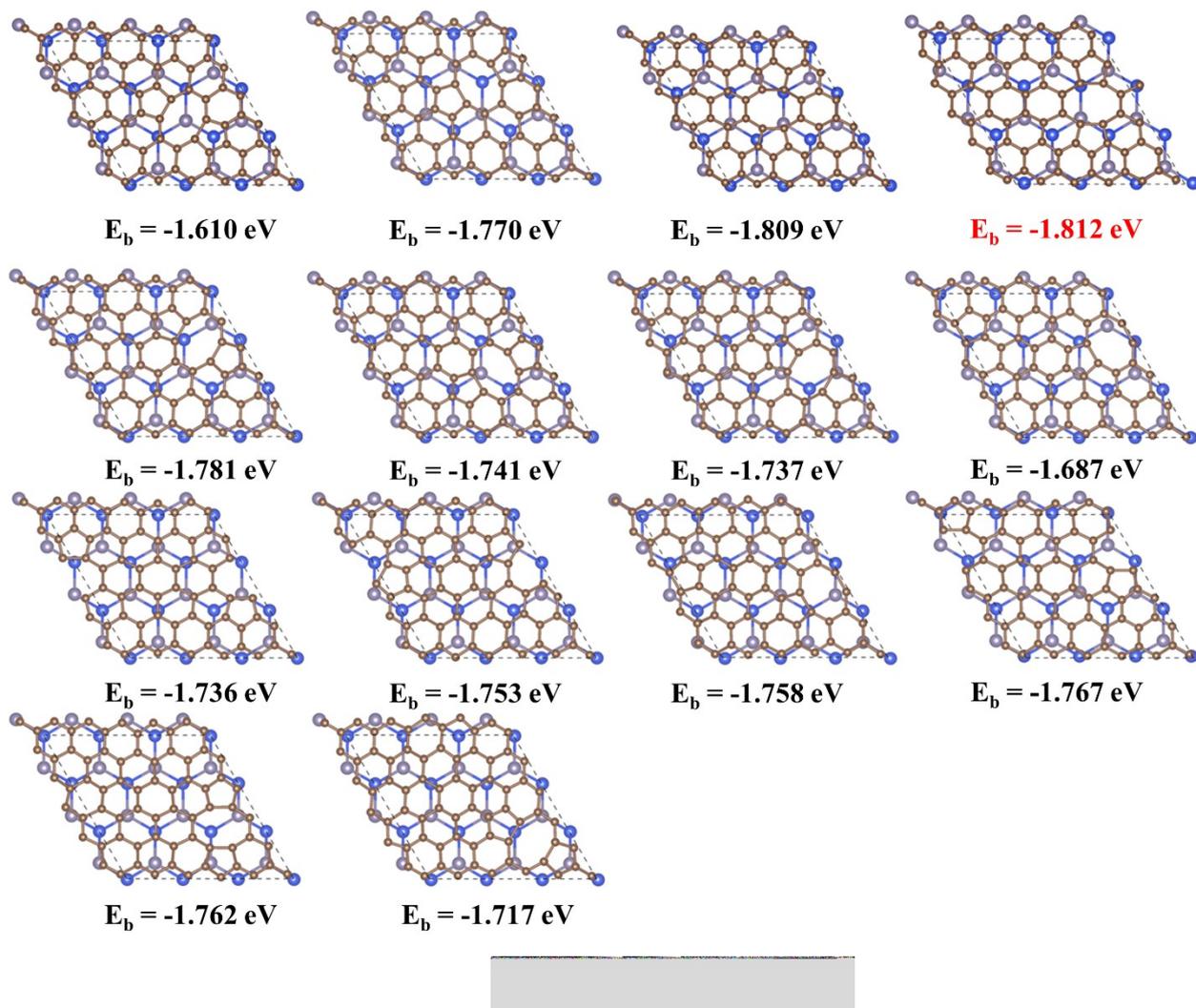[b] *School of Energy and Power Engineering, Chongqing University, Chongqing 400044, China*

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$E_b = -2.322$ eV $E_b = -2.055$ eV $E_b = -2.291$ eV $E_b = -0.691$ eV

$E_b = -0.712$ eV $E_b = -0.694$ eV $E_b = -0.713$ eV $E_b = -0.693$ eV

$E_b = -2.317$ eV $E_b = -0.705$ eV $E_b = -2.314$ eV $E_b = -0.695$ eV

$E_b = -2.310$ eV

○ Ge   ● Si   ○ C

Figure S1 SV-G/S configurations based on symmetry considerations (E_b represents the binding energy).

$E_b = -1.610$ eV $E_b = -1.770$ eV $E_b = -1.809$ eV $E_b = -1.812$ eV

$E_b = -1.781$ eV $E_b = -1.741$ eV $E_b = -1.737$ eV $E_b = -1.687$ eV

$E_b = -1.736$ eV $E_b = -1.753$ eV $E_b = -1.758$ eV $E_b = -1.767$ eV

$E_b = -1.762$ eV $E_b = -1.717$ eV

Figure S2 DV-G/S configurations based on symmetry considerations. (E_b represents the binding energy).

$E_b = -0.884$ eV $\qquad$ $E_b = -0.864$ eV $\qquad$ $E_b = -0.864$ eV $\qquad$ $E_b = -0.694$ eV

$E_b = -0.788$ eV $\qquad$ $E_b = -0.770$ eV $\qquad$ $E_b = -0.817$ eV $\qquad$ $E_b = -0.837$ eV

$E_b = -0.864$ eV $\qquad$ $E_b = -0.864$ eV $\qquad$ $E_b = -0.888$ eV $\qquad$ $E_b = -0.796$ eV
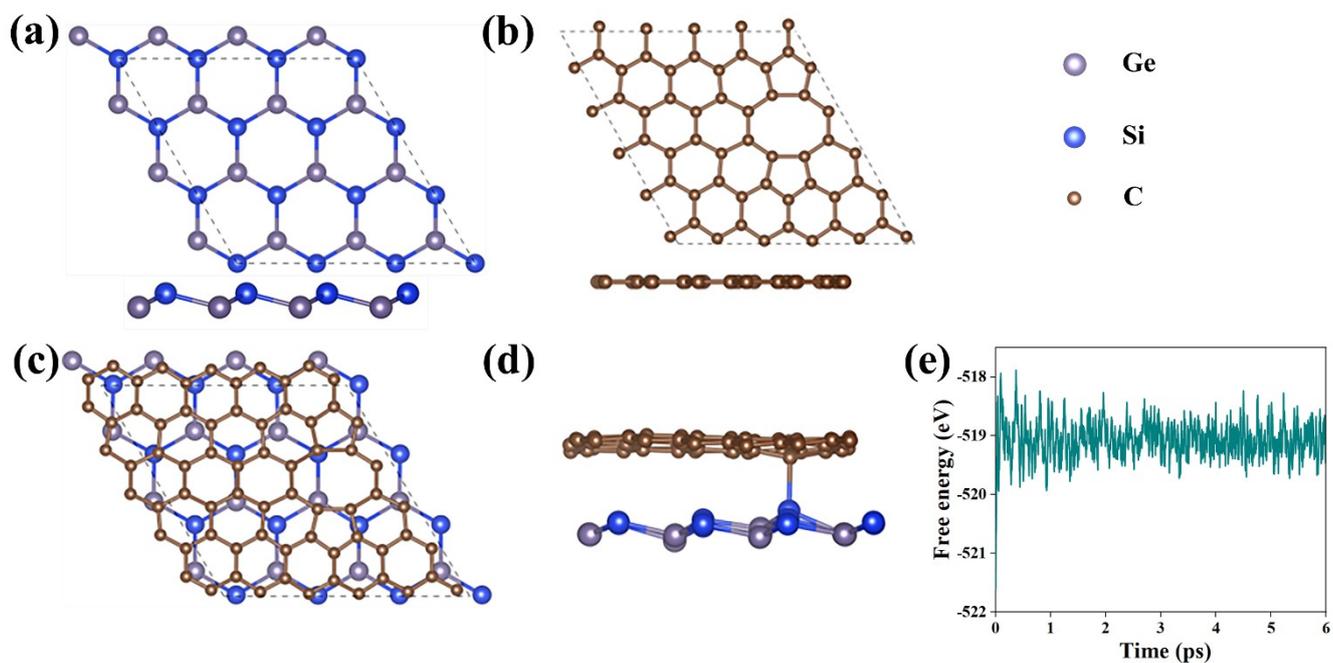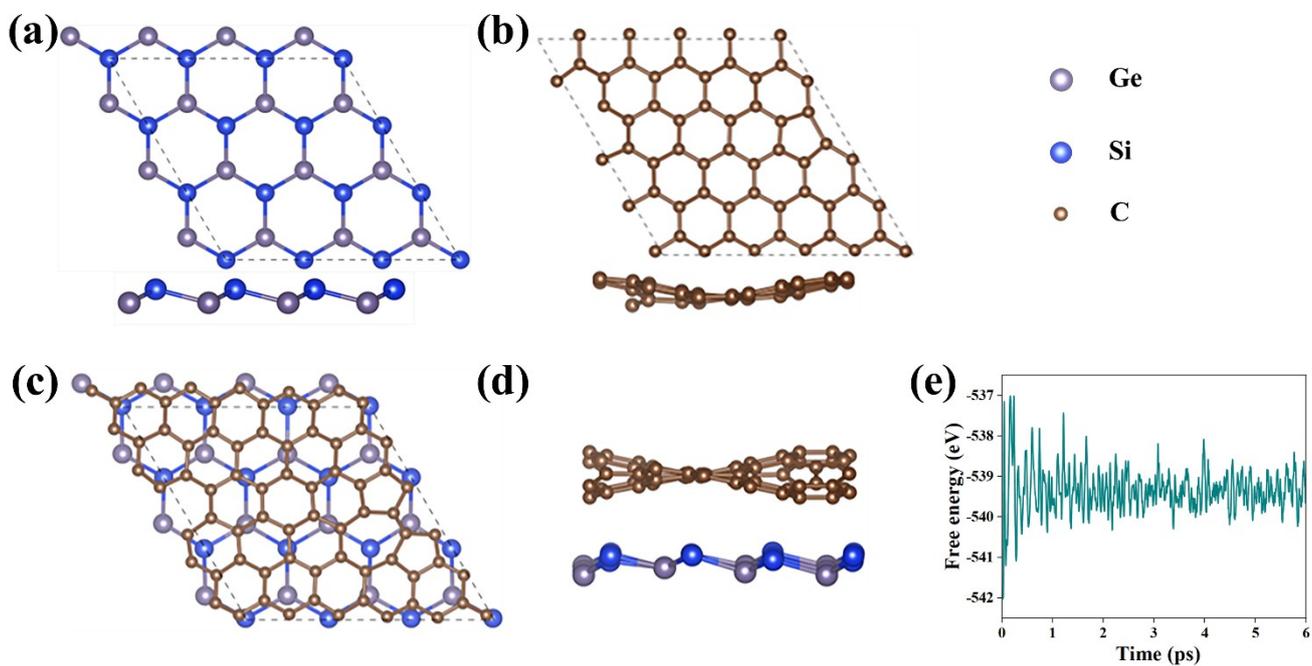
$E_b = -0.834$ eV $\qquad$ $E_b = -0.805$ eV
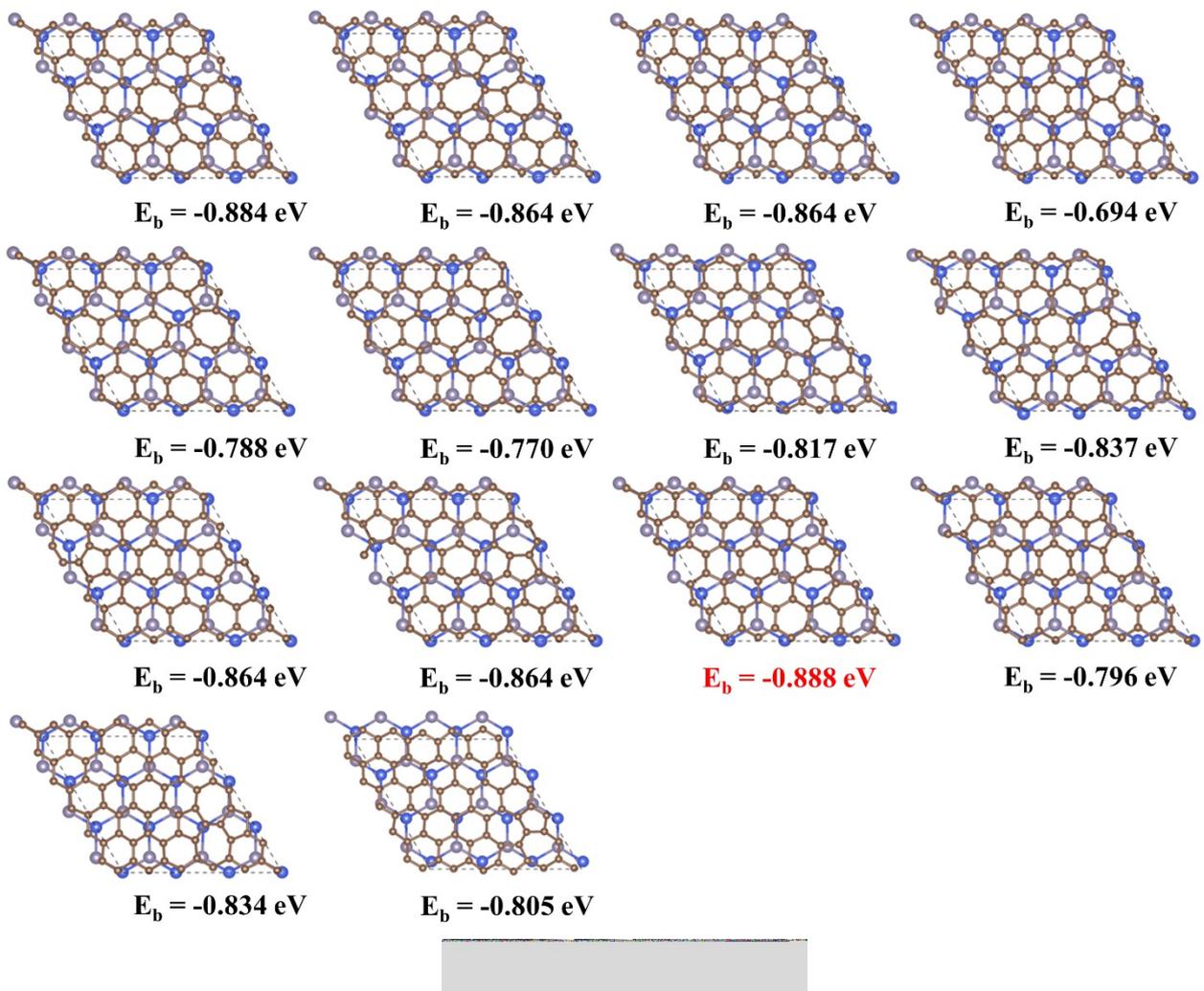
Figure S3 SW-G/S configurations based on symmetry considerations. (E_b represents the binding energy).

Figure S4 (a) Top and side views of the structure of 2D SiGe. **(b)** Top and side views of the structure of graphene with DV defect. **(c)** Top and **(d)** side view the structure of DV-G/S. **(e)** Free Energy as a function of MD time at a temperature of 300K for DV-G/S.

Figure S5 (a) Top and side views of the structure of 2D SiGe. **(b)** Top and side views of the structure of graphene with SW defect. **(c)** Top and **(d)** side view the structure of SW-G/S. **(e)** Free Energy as a function of MD time at a temperature of 300K for SW-G/S.
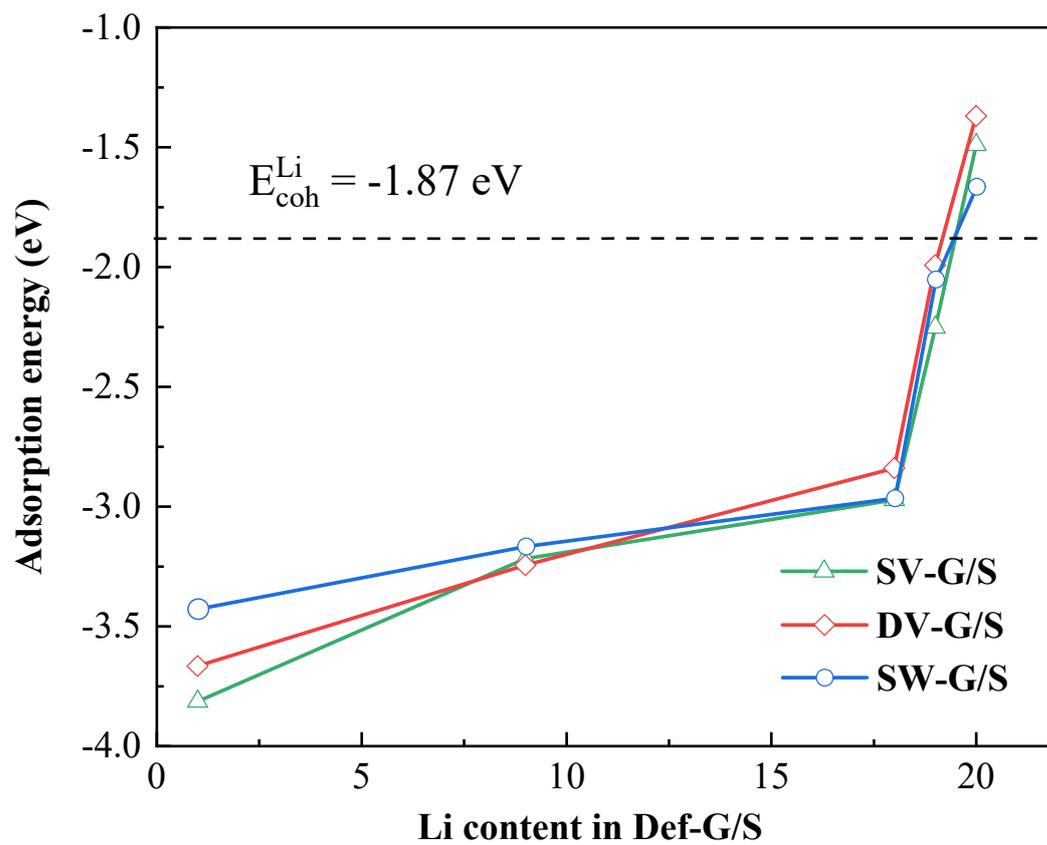
Figure S6 Li adsorption energies of SV-G/S, DV-G/S and SW-G/S as a function of Li adsorption concentration.

Table S1 Adsorption energies (eV) for Li adsorbed at each possible adsorption site on the top, middle and bottom of Def-G/S.

Adsorption site	SV-G/S			DV-G/S			SW-G/S		
	top	middle	bottom	top	middle	bottom	top	middle	bottom
1	-2.41	-3.58	-3.18	-2.44	-3.56	-3.11	-2.15	-3.33	-2.95
2	-2.39	-3.65	-3.18	-2.40	-3.45	-3.09	-2.16	-3.40	-2.92
3	-2.46	-3.25	-3.16	-2.40	-3.57	-3.14	-2.20	-3.33	-2.91
4	-2.54	-3.71	-3.19	-2.42	-3.57	-3.10	-2.20	-3.35	-2.91
5	-2.57	-3.81	-3.21	-2.45	-3.54	-3.15	-2.19	-3.43	-2.93
6	-2.41	-3.24	-3.16	-2.57	-3.67	-3.14	-2.23	-3.43	-2.92
7	-2.40	-3.71	-3.19	-2.42	-3.51	-3.12	-2.20	-3.29	-2.90
8	-2.66	-3.65	-3.18	-2.44	-3.66	-3.15	-2.17	-3.42	-2.93
9	-3.05	-3.51	-3.14	-2.56	-3.61	-3.13	-2.15	-3.07	-2.87
10	-3.05	-	-	-2.63	-	-	-2.22	-	-
11	-2.42	-	-	-2.53	-	-	-2.49	-	-
12	-2.50	-	-	-2.45	-	-	-2.22	-	-
13	-2.80	-	-	-2.57	-	-	-2.17	-	-
14	-3.05	-	-	-2.92	-	-	-2.30	-	-
15	-2.56	-	-	-2.41	-	-	-2.40	-	-
16	-2.40	-	-	-2.42	-	-	-2.38	-	-
17	-2.50	-	-	-2.61	-	-	-2.19	-	-
18	-2.66	-	-	-2.72	-	-	-2.20	-	-
19	-2.54	-	-	-2.61	-	-	-2.46	-	-
20	-2.44	-	-	-2.36	-	-	-2.48	-	-
21	-2.42	-	-	-2.48	-	-	-2.29	-	-
22	-2.41	-	-	-2.48	-	-	-2.17	-	-
23	-2.46	-	-	-2.48	-	-	-2.23	-	-
24	-2.45	-	-	-2.39	-	-	-2.30	-	-
25	-2.44	-	-	-	-	-	-2.47	-	-
Mean value	-2.56	-3.57	-3.18	-2.51	-3.57	-3.13	-2.27	-3.34	-2.91

Table S2 Average charge transfer of Li($\mathit{\Delta Q}_{Li}$), top (ΔQ_{Gra}) and bottom (ΔQ_{SiGe}) in DV-G/S, A positive/negative $\mathit{\Delta Q}$ denote a loss/gain of electrons.

System	$\mathit{\Delta Q}_{Li}$	$\mathit{\Delta Q}_{SiGe}$	$\mathit{\Delta Q}_{Gra}$
Li/Gra/SiGe	+0.79	-1.34	+0.55
Gra/Li/SiGe	+0.44	-0.96	+0.52
Gra/SiGe/Li	+0.43	-0.90	+0.47

Table S3 Average charge transfer of Li($\mathit{\Delta Q}_{Li}$), top (ΔQ_{Gra}) and bottom (ΔQ_{SiGe}) in SW-G/S, A positive/negative $\mathit{\Delta Q}$ denote a loss/gain of electrons.

System	$\mathit{\Delta Q}_{Li}$	$\mathit{\Delta Q}_{SiGe}$	$\mathit{\Delta Q}_{Gra}$
Li/Gra/SiGe	+0.76	-1.11	+0.36
Gra/Li/SiGe	+0.36	-0.67	+0.30
Gra/SiGe/Li	+0.40	-0.62	+0.22