Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

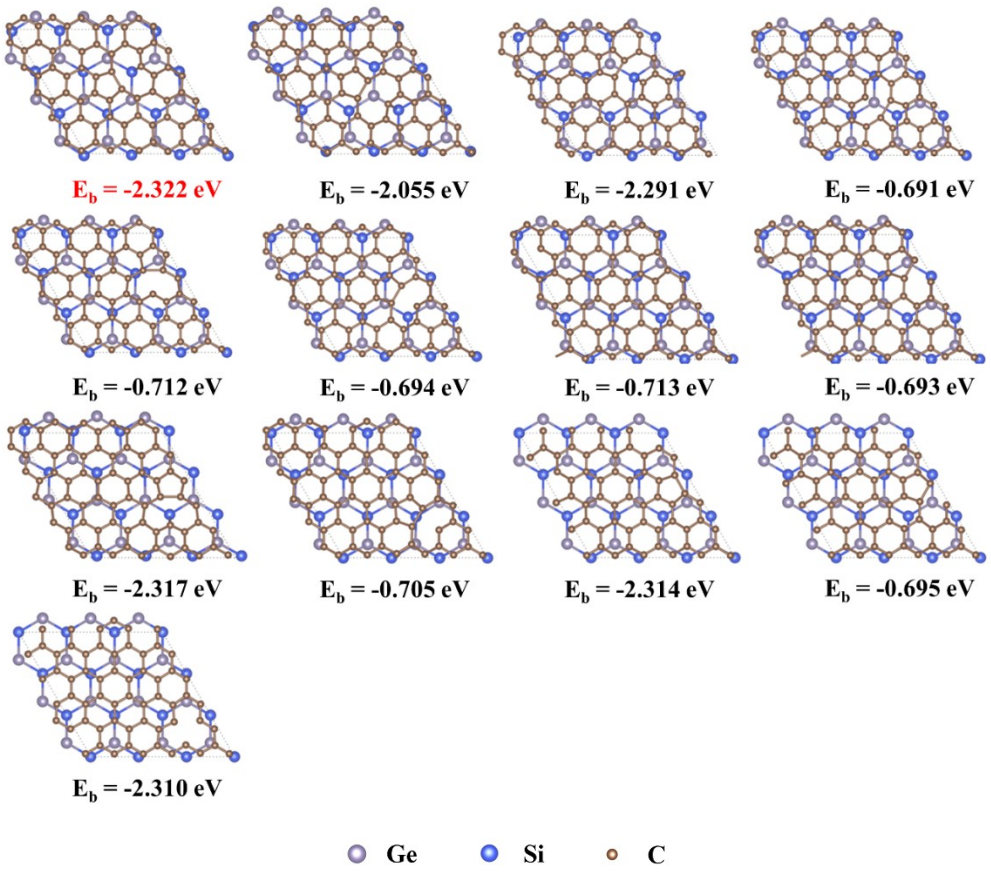

Figure S1 SV-G/S configurations based on symmetry considerations (E_b represents the binding energy).

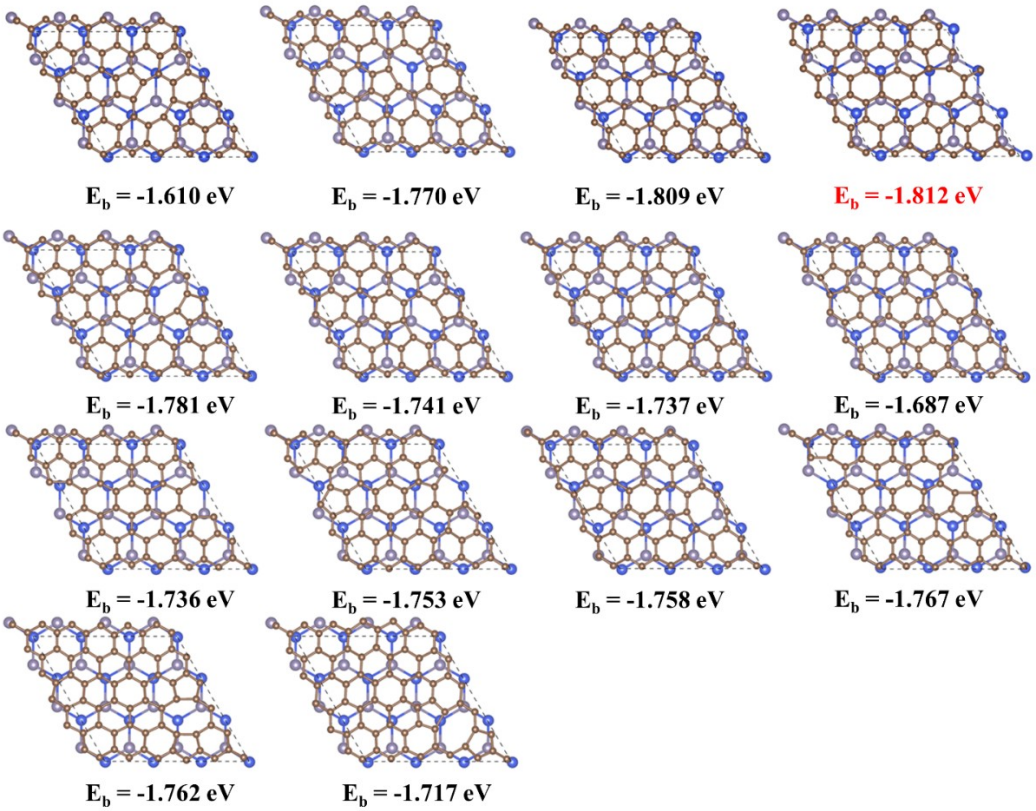

Figure S2 DV-G/S configurations based on symmetry considerations. (E_b represents the binding energy).

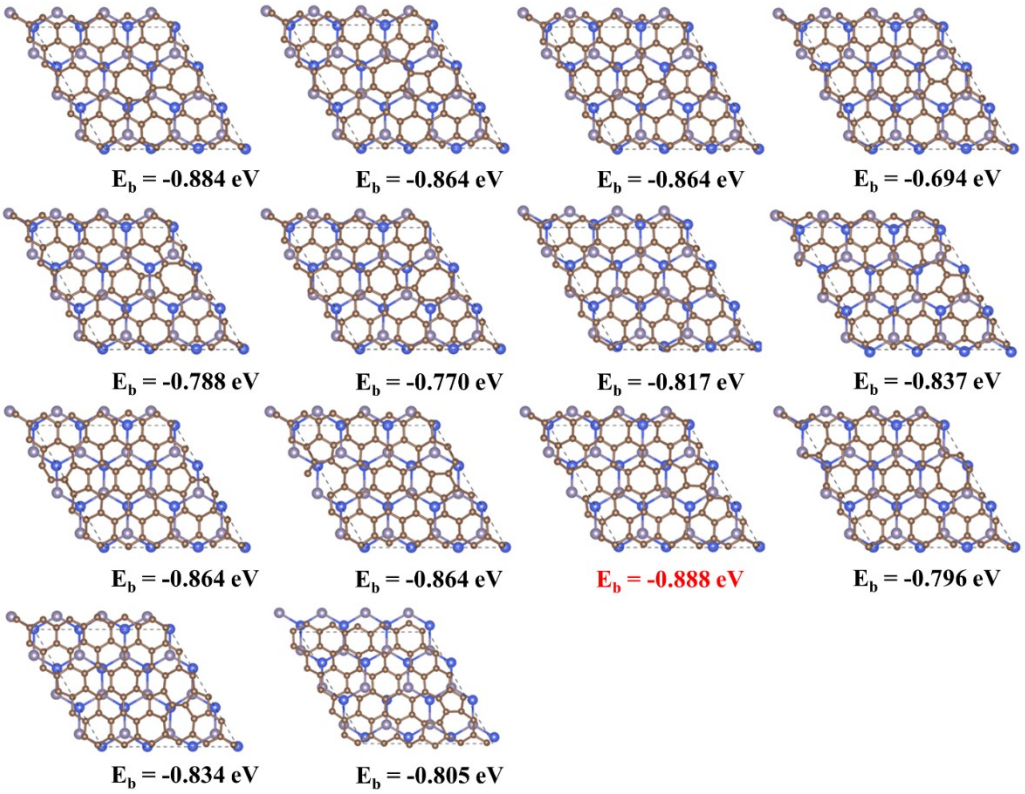

Figure S3 SW-G/S configurations based on symmetry considerations. (E_b represents the binding energy).

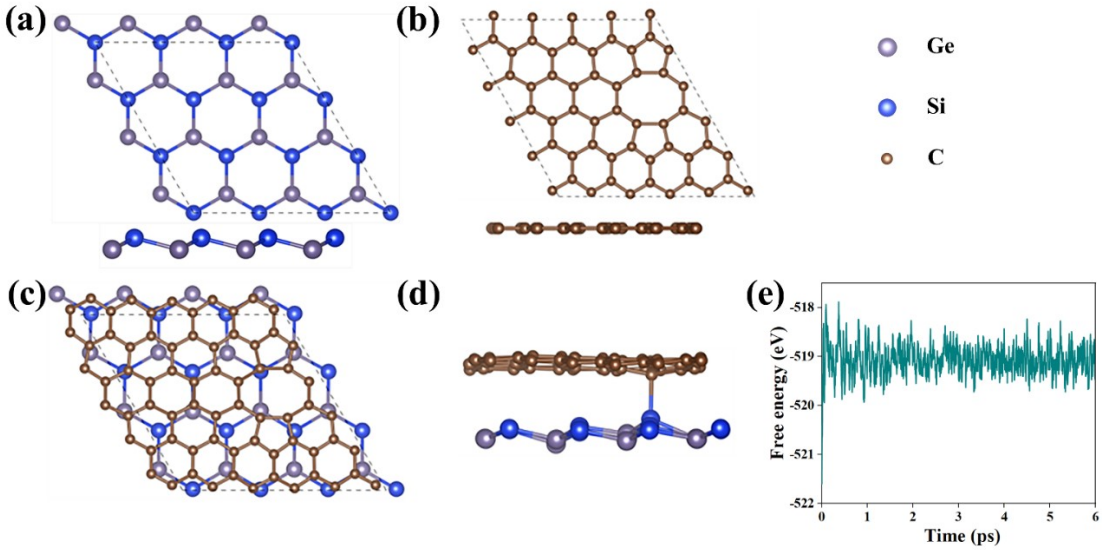

Figure S4 (a) Top and side views of the structure of 2D SiGe. **(b)** Top and side views of the structure of graphene with DV defect. **(c)** Top and **(d)** side view the

structure of DV-G/S. **(e)** Free Energy as a function of MD time at a temperature of 300K for DV-G/S.

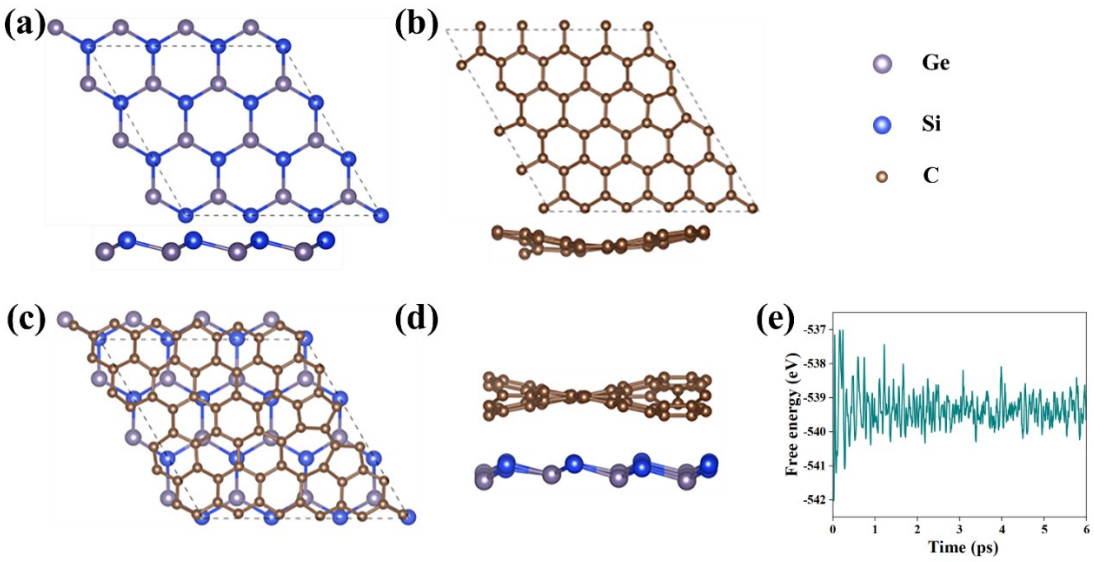

Figure S5 (a) Top and side views of the structure of 2D SiGe. **(b)** Top and side views of the structure of graphene with SW defect. **(c)** Top and **(d)** side view the structure of SW-G/S. **(e)** Free Energy as a function of MD time at a temperature of 300K for SW-G/S.

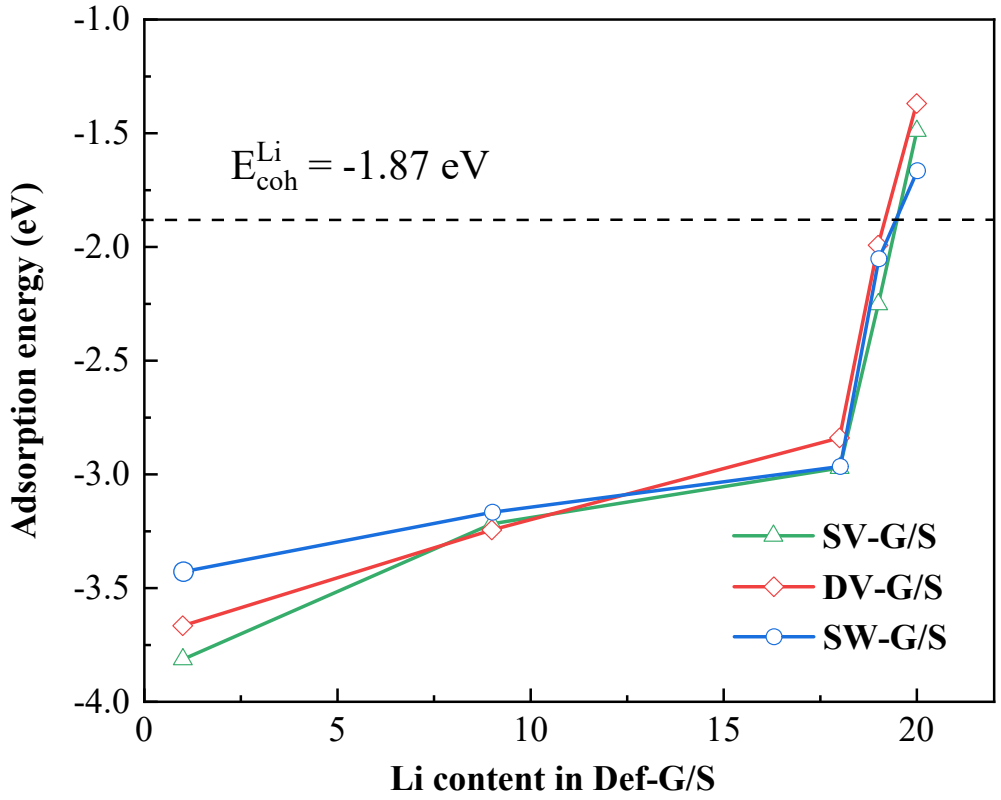

Figure S6 Li adsorption energies of SV-G/S, DV-G/S and SW-G/S as a function of Li adsorption concentration.