

Supporting Information

for

Coexistence of strongly buckled germanene phases on Al(111)

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Detailed information of the (3×3) and ($\sqrt{7}\times\sqrt{7}$) models

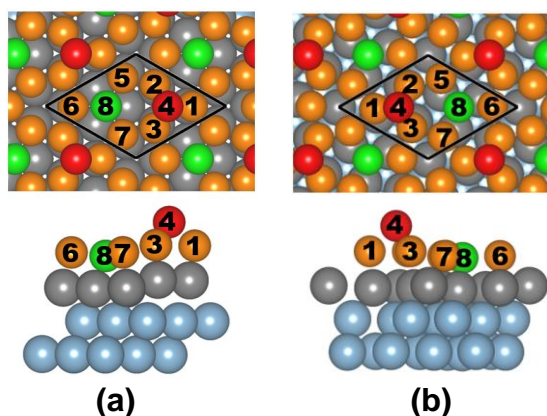


Figure S1: (a) Top and side views of the relaxed model of (2×2) germanene on (3×3) Al(111). The black cell represents a (3×3) reconstruction with respect to the Al(111) surface. (b) Top and side views of the relaxed model of (2×2) germanene on ($\sqrt{7}\times\sqrt{7}$) Al(111). The black cell represents a ($\sqrt{7}\times\sqrt{7}$) reconstruction with respect to the Al(111) surface.

In the 3×3 model, the bond lengths and angles between Ge(4) and Ge(1-3) are ~ 2.56 Å and $\sim 81.0^\circ$, respectively; the bond lengths and angles between Ge(8) and Ge(5-7) are ~ 2.52 Å and $\sim 118.5^\circ$, respectively; The adsorption energy is -0.45 eV/Ge atom.

In the $\sqrt{7}\times\sqrt{7}$ model, the bond lengths and angles between Ge(4) and Ge(1-3) are ~ 2.55 Å and $\sim 78.0^\circ$, respectively; the bond lengths and angles between Ge(8) and Ge(5-7) are ~ 2.55 Å and $\sim 120.0^\circ$, respectively; The adsorption energy is -0.46 eV/Ge atom.

The charge transfer is calculated by the Bader scheme within VASP.

The germanene layer gains totally 1.80 and 2.32 electrons in the 3×3 and $\sqrt{7}\times\sqrt{7}$ models, respectively, from Al atoms. In the 3×3 model, Ge(8) gains 0.40 electron; Ge(5-7) gain 0.33-0.34 electron/atom; Ge(1-3) gain 0.18-0.19 electron/atom; Ge(4) loses 0.15 electron. The charge transfer calculation of the $\sqrt{7}\times\sqrt{7}$ model: Ge(5-7) gain 0.38-0.41 electron/atom; Ge(1-3,8) gain 0.31-0.32 electron/atom; Ge(4) loses 0.14 electron.

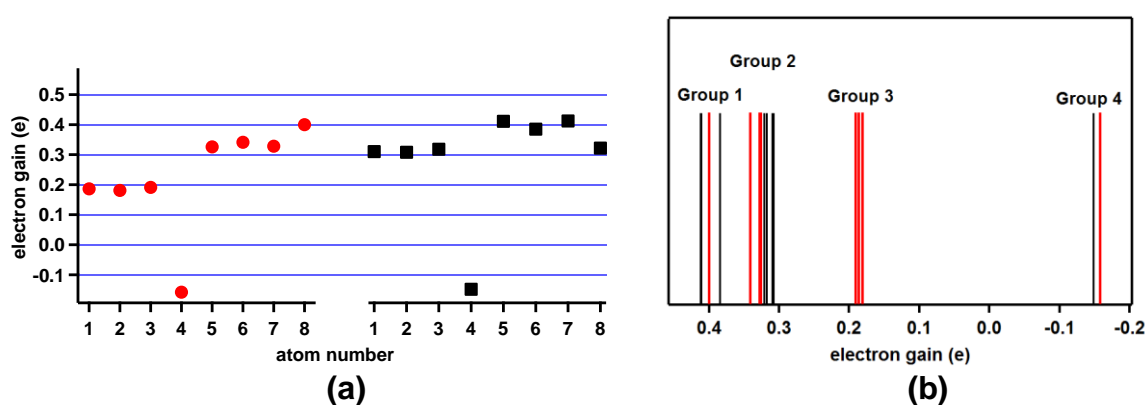


Figure S2: (a) Charge transfer diagram for different Ge atoms of the 3×3 (red dots) and the $\sqrt{7}\times\sqrt{7}$ (black squares) models in Figure S1. (b) The grouping is based on the quantity of electron gain. The red and black bars correspond to the 3×3 and the $\sqrt{7}\times\sqrt{7}$ models respectively. Note that there is no Ge atom of the $\sqrt{7}\times\sqrt{7}$ model with a charge similar to the group 3 atoms of the 3×3 model.