Supplementary Information

Direct Formation of Large-Scale Multi-Layered Germanene on Si Substrate

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1 Layer

2 Layers

sp³ bonding
(2.401 Å)

3 Layers

sp³-like bonding
(2.408 Å)

4 Layers
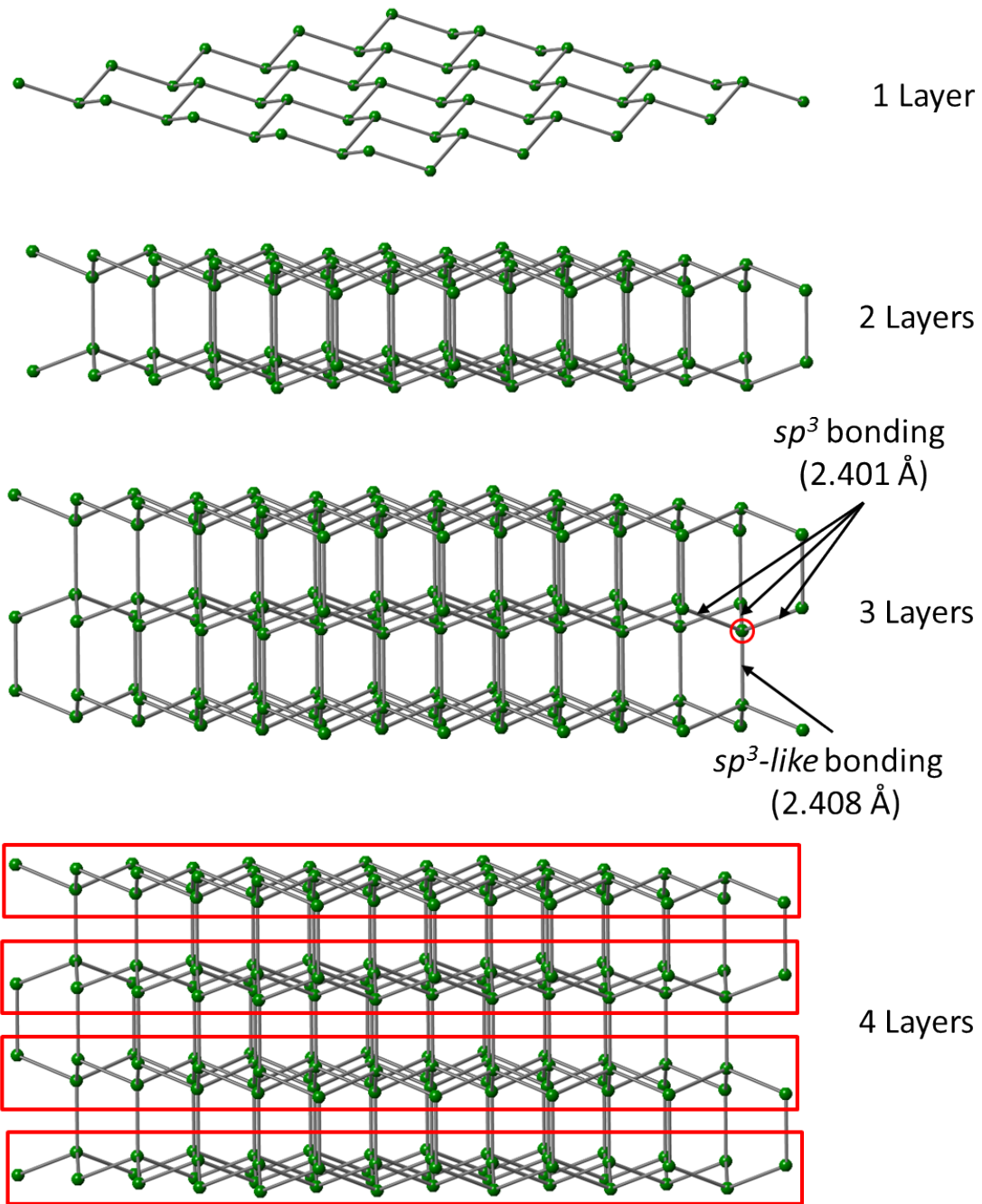
Figure S1. The lonsdaleite Ge crystal structure with *sp³*–*sp³*-like mixed orbital hybridization.

Calculation: The diffraction pattern in Fig. 3c could be used to calculate the interplanar distances. In Supplementary Fig. 2a, the length of green dash line, which contains double reciprocal vector, is equal to 10.09 nm^{-1}, so that the length of reciprocal vector is 5.045 nm^{-1}. The inverse of 5.045 nm^{-1} is equal to 0.198 nm that is the interplanar distance of particular planes. In Ref. 1, the computational result indicates the lattice constant (a) of lonsdaleite germanium is 0.392 nm. The (11-20) interplanar distance is actually equal to a/2 (0.196 nm) which is consistent with the value from our calculation. On the other hand, the length (13.06 nm^{-1}) of blue dash line as shown in Supplementary Fig. 2b contains quadruple reciprocal vector. Hence the length of reciprocal vector is 3.265 nm^{-1}. The inverse of 3.265 nm^{-1} is equal to 0.306 nm. In lonsdaleite structure, the c/a ratio is 1.64[2] so that the c value (0.642 nm) of germanene is the product of 0.392 and 1.64. In the equilibrium state, the (0002) interplanar distance (d) is equal to c/2[1], which is 0.321 nm. This calculation result is in agreement with that of experiment and the error is less than 5%, indicating that the results are believable.
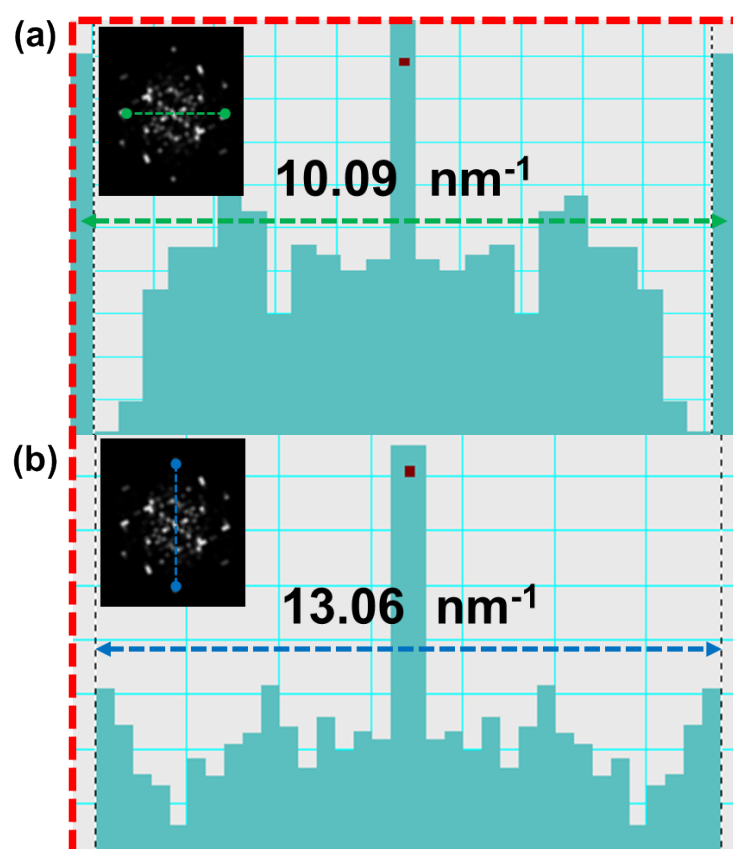
Figure S2. (**a**) The distance between (11-20) reciprocal points, (**b**) The distance between (0002) reciprocal points.

References

1. S. Wang, *Phys. Chem. Chem. Phys.,* 2011, **13**, 11929.

2. http://en.wikipedia.org/wiki/Lonsdaleite