Supplementary information

Exploring Ag(111) Substrate for Epitaxially Growing Monolayer Stanene: A First-Principles Study

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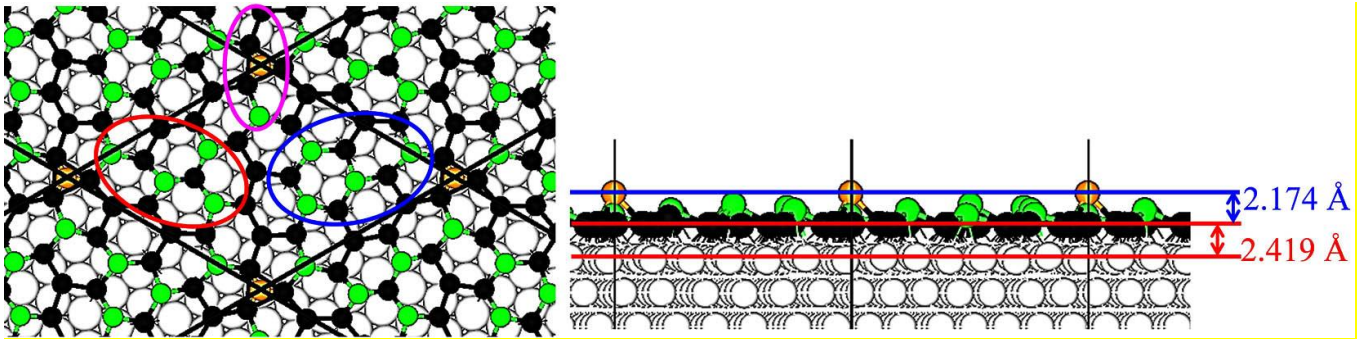

Figure S1. Optimized structure of the supercell containing a $(4 \times 4)R0°$ stanene on a $(\sqrt{43} \times \sqrt{43})R7.589°$ Ag(111), with dimensions of 19.229 Å × 19.229 Å × 25.000 Å. The bucking pattern of this large supercell can be recognized as a mixture of S1 (blue circle), S2 (red circle) and S3 (purple circle) structures (see Fig 1 in the main text). The binding energy between this stanene structure and Ag (111) surface is -0.058 eVÅ^{-2}, and the height of the low-level Sn atoms (black balls) to Ag(111) surface is about 2.419 Å. Both the binding energy E_b and the average height $\bar{d}$ are between those of S1(S2) and S3. The highest buckling point of this stanene structure is 2.174 Å.

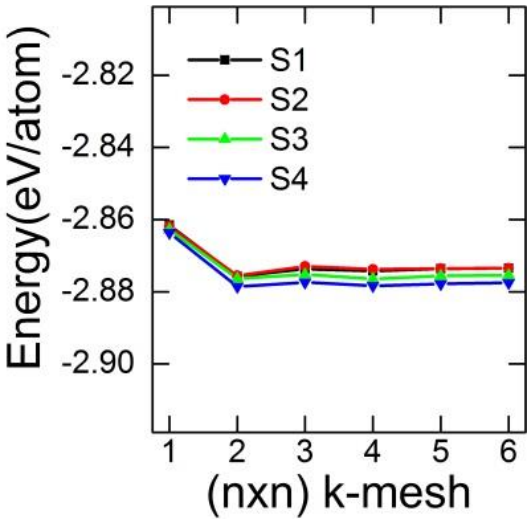

Figure S2. The K-mesh test for the structural relaxation of $(\sqrt{7} \times \sqrt{7})R19.107°$ stanene on $(\sqrt{19} \times \sqrt{19})R23.413°$ Ag(111) supercell. It is found the (2×2×1) k-mesh used in our calculations can give good energy convergence for structural relaxations; the order of stability of S1-S4 is the same as that from calculations adopted the (6×6×1) k-mesh.