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Supplementary

Ultrathin β-tellurium layers grown on highly oriented pyrolytic graphite by molecular-beam epitaxy

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S1. Auger Electron Spectroscopy of the grown sample

Measurements by Auger Electron Epectroscopy (AES) have been performed to show the composition of the deposited films. Figure S1 below shows a typical result, which reveals two groups of AES peaks as marked by the red and green arrows in (a). Figure S1 (b) and (c) are spectra taken over narrow ranges of energies, highlighting the two groups of AES peaks. The red curve in (b) shows the peak at energy ~275 eV, which is from C of the HOPG substrate. The green curve in (c) shows two peaks at ~486 eV and ~494 eV, respectively, which signifies elemental tellurium of the deposit. In the spectra, no other peak is apparent, suggesting that the deposit in our MBE experiment is of pure Te.

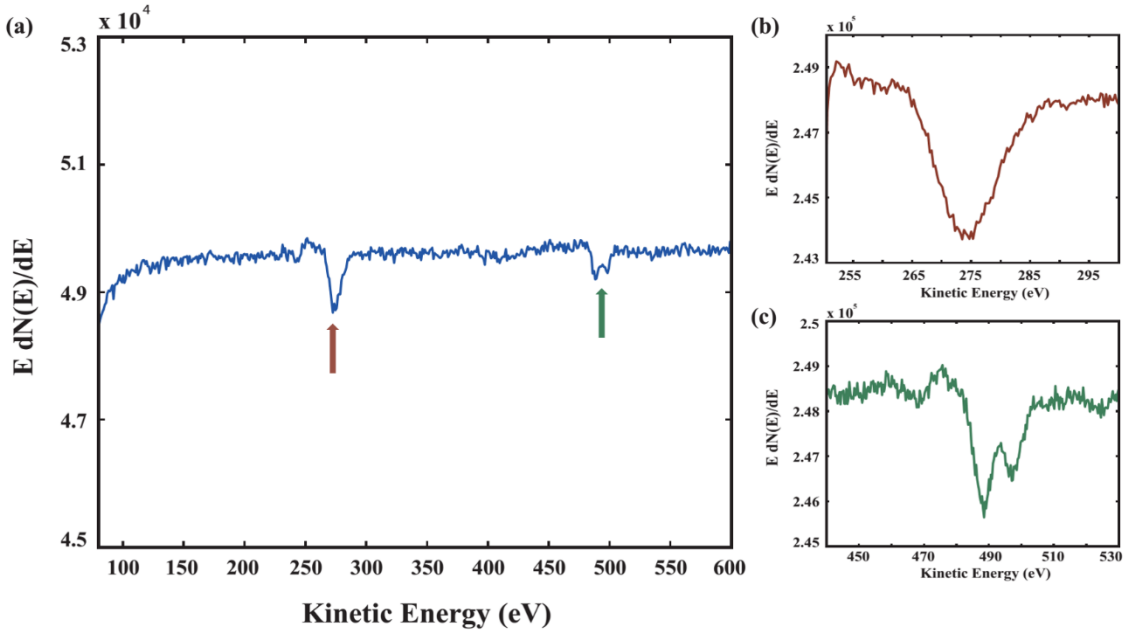

Figure S1. (a) AES over a large energy range (75 eV~600 eV) of a grown sample. The red and green arrows point two groups of AES peaks seen in the spectrum corresponding to C and Te respectively. (b) A close-up spectrum over a narrow energy range covering the red-arrow pointed peak at ~275 eV in (a). (c) A close-up spectrum at energies close to the green-arrow pointed peaks in (a). The two peaks at ~486 and ~494 eV signify elemental Te in sample.

S2. Mound growth of Te on HOPG and calibration of Te epifilm thickness

Te tends to grow in mounds of multi-layer high on HOPG, leaving some areas of the substrate surface exposed. The Figures below show two large scale STM micrographs, which reveal the tall mounds on the right and the exposed HOPG surface on the left. This morphology allowed us to calibrate the thickness of the epitaxial Te films by STM line-profiling (see inset). From high-resolution STM images, such as that of Fig. 1c in the main text, we can derive the step height or the height of monolayer Te, so the height of different terraces may be derived. At the bottom of the mound, one may discern small terraces of monolayer and bilayer Te as well.

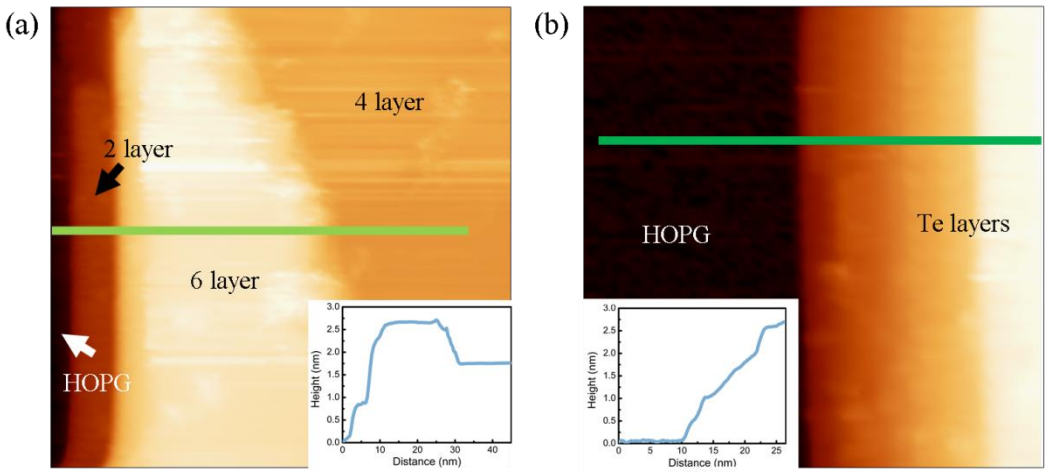

Figure S2. (a) and (b) are STM images (size: 50×50 nm^2, bias: 0.8V) showing a Te mound (right bright contrast) on HOPG (left dark contrast). Inset show the line profiles taken along the green lines drawn.

S3. STM of a thick Te epilayer

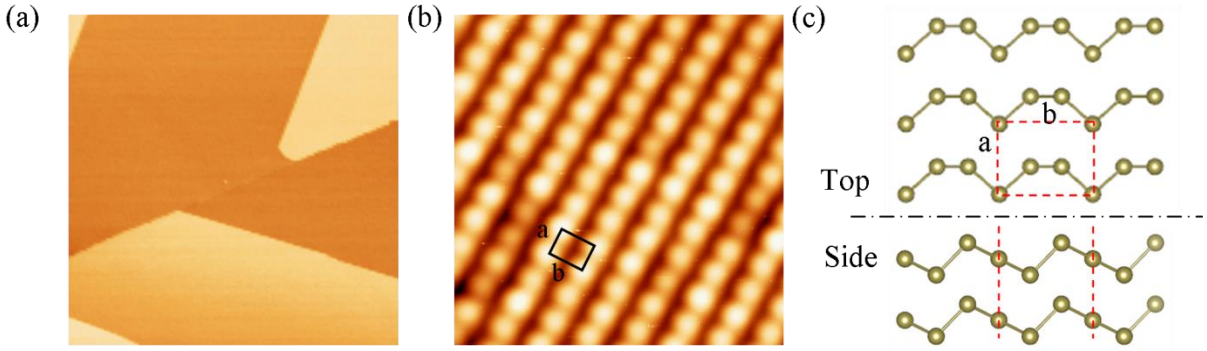

Figure S3. (a) STM topographic image of a thick Te film (≥ 80 Å) grown on HOPG (size: 100×100 nm^2, bias: 1V). (b) An atomic resolution image of the same surface, revealing a lattice size of 5.91×4.33 $Å^2$ under the bias of 1V (marked by the rectangle). (c) Stick-and-ball model of the bulk Te viewed from top and side, respectively. The dash lines mark the surface unit cell.

S4. Partial charge density distribution of double and triple layers of β-tellurene

Figure (a) and (b) below present the charge density distributions at the energy of (a) CBM and (b) VBM for a double (left) and triple (right) β-tellurene layers (all isosurfaces are set at 0.04 eÅ^{-3}). Figures (c) and (d) are for that of a helical phase Te of the same thicknesses. It can be seen that for β-phase Te, the partial charge density at CBM is very much confined in the middle atom layer and that at VBM extends out from the top and bottom layers of Te, therefore the latter would suffer from the coupling effect more strongly. For the helical-phase Te, a totally different characteristics can be observed.

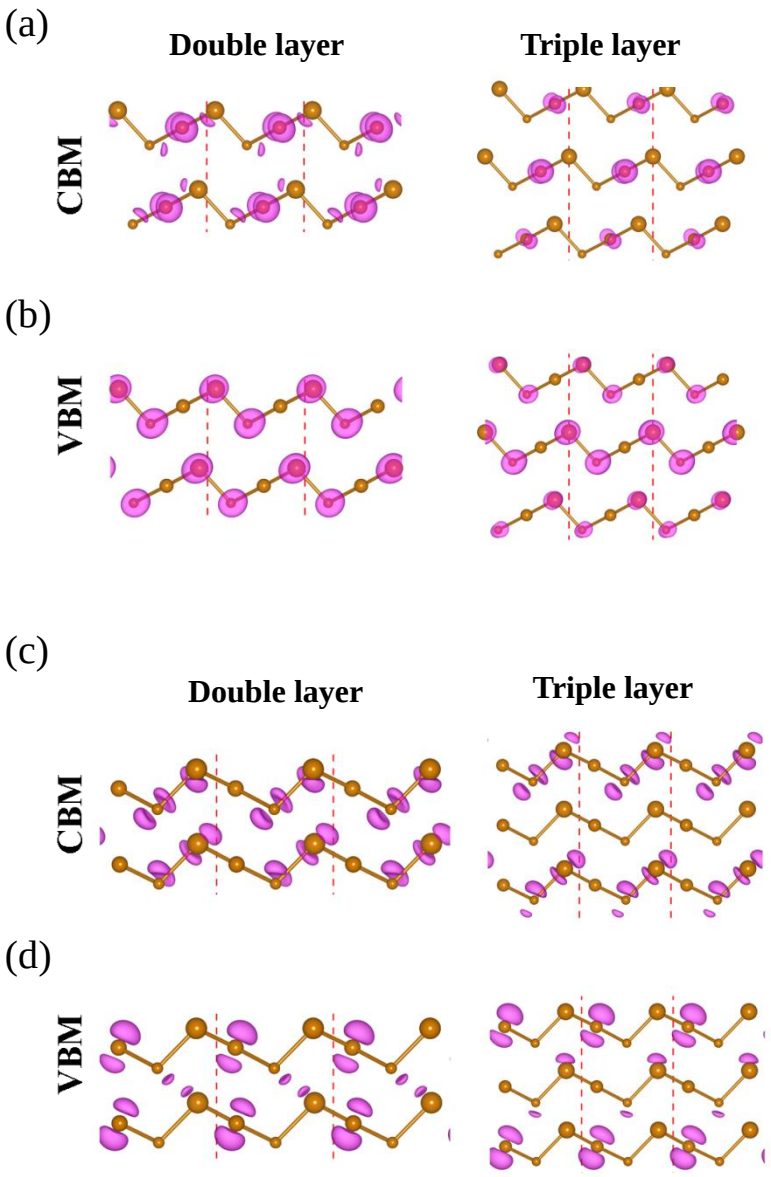

Figure S4. Partial charge density distribution of (a) CBM and (b) VBM for a double (left) and triple (right) β-tellurene layers (all isosurfaces are set to 0.04 eÅ^{-3}). Figures (c) and (d) are for that of a helical phase Te.

S5. Band structures of single, double and triple layer of β-Te

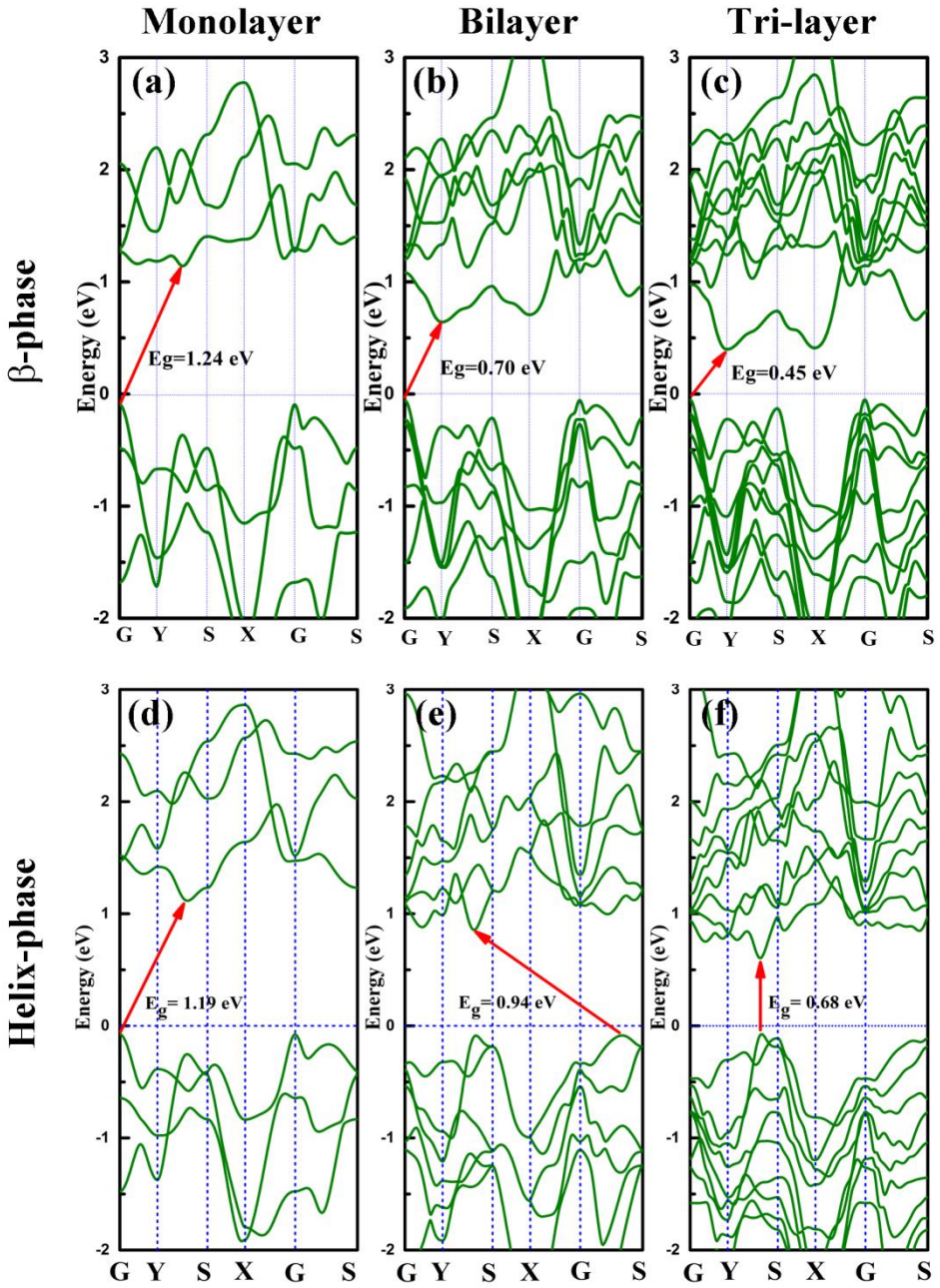

Figure S5. (a-c) are the DFT calculated band structures for of a single, double and triple β-Te layer. For comparison, Figures (d-f) are the band structures of the helical phase Te for the similar thicknesses.