Supplementary Information

Diverse electronic properties of 2D layered Se-containing materials composed of quasi-1D atomic chains

Yawen Li[a], Yuanhui Sun[a], Guangren Na[a], Wissam A. Saidi[b,] and Lijun Zhang[a,]**

[a]Key Laboratory of Automobile Materials of MOE and School of Materials Science and Engineering, Jilin University, Changchun, 130012, China
[b]Department of Mechanical Engineering and Materials Science, University of Pittsburgh, Pittsburgh, Pennsylvania 15261, USA

E-mail: alsaidi@pitt.edu, lijun_zhang@jlu.edu.cn

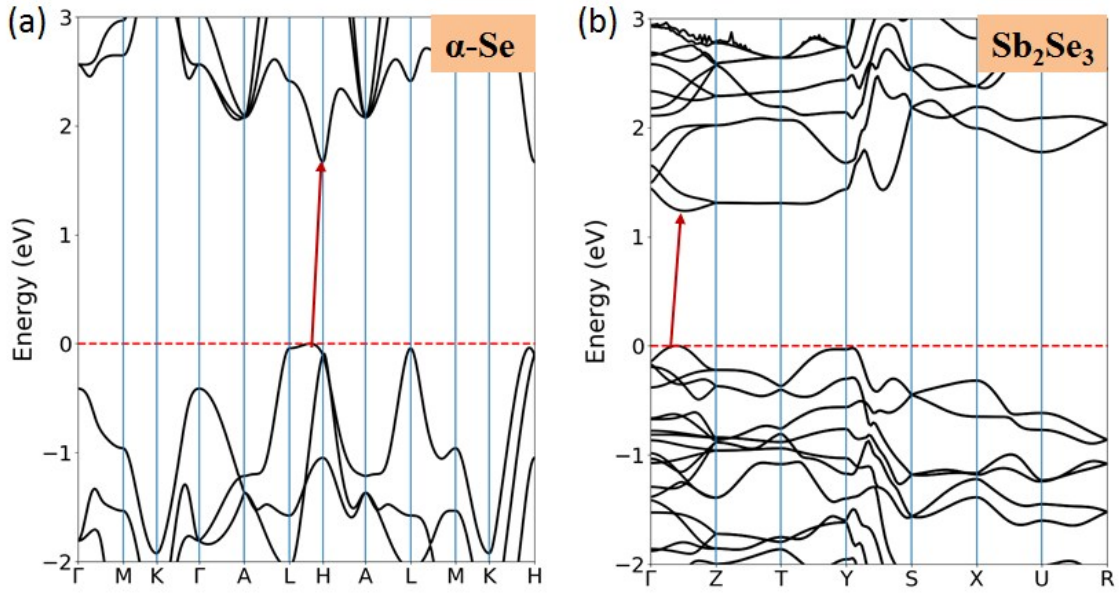

Figure S1. The HSE functional calculated band structure of bulk α-Se and Sb_2Se_3. Both bulk α-Se and Sb_2Se_3 are indirect band gap semiconductors. The spin orbital coupling is considered.

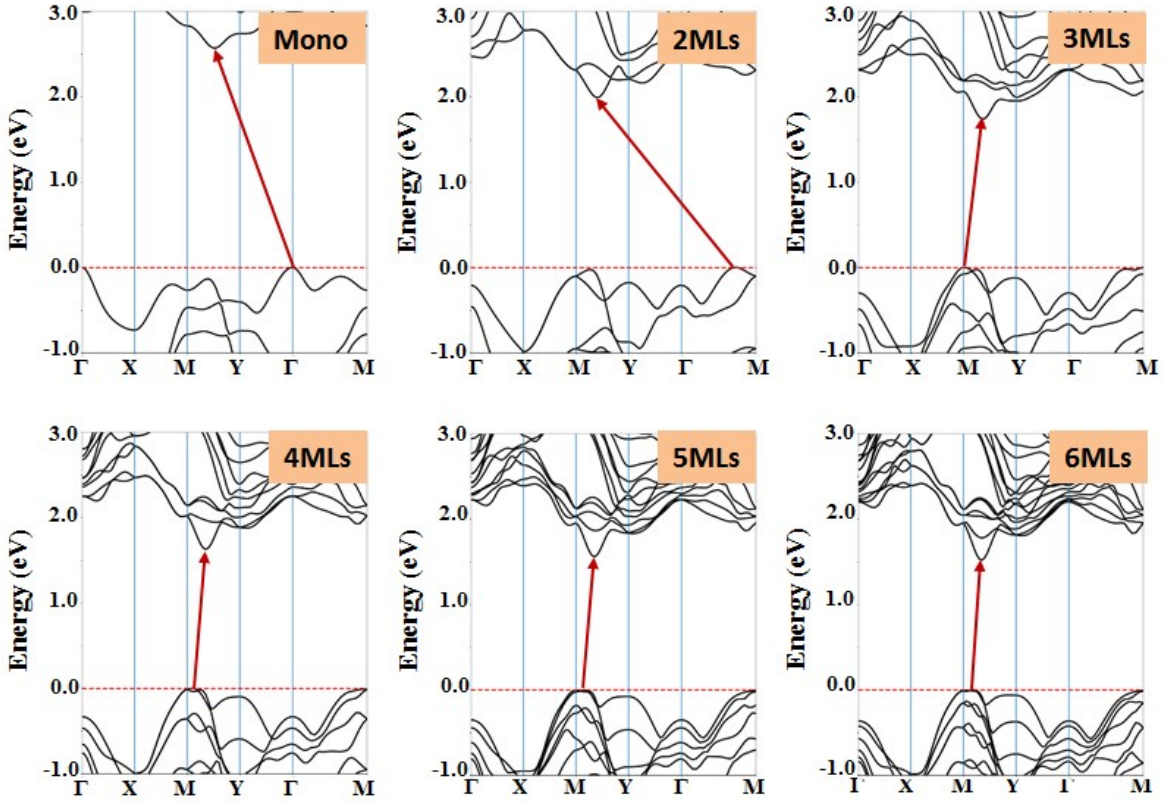

Figure S2. The HSE functional calculated band structures of α-Se from n=1 to n=6.

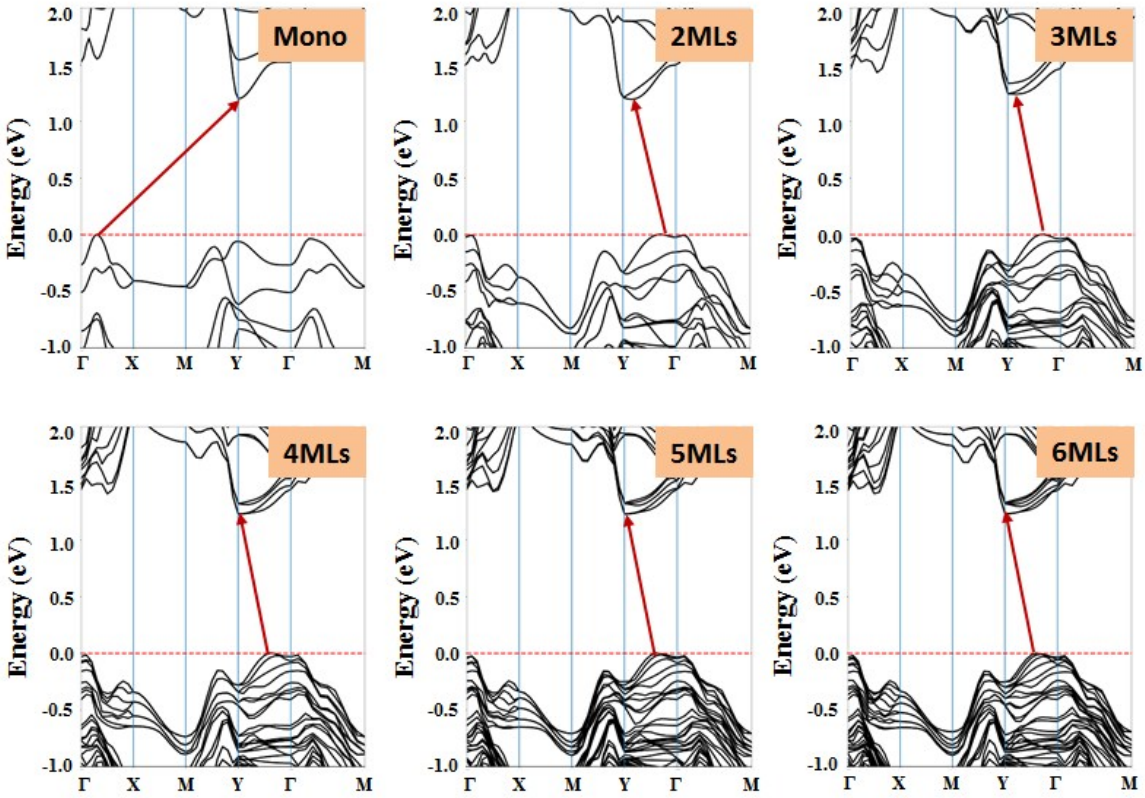

Figure S3. The HSE functional calculated band structures of Sb_2Se_3 from n=1 to n=6.

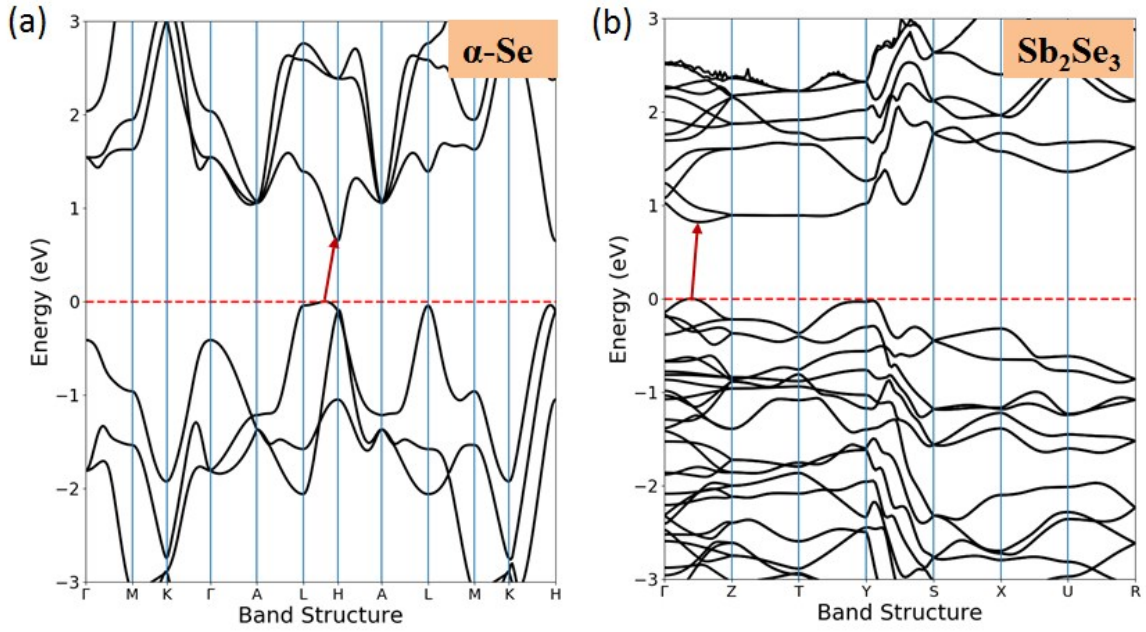

Figure S4. PBE band structure of bulk α-Se and Sb_2Se_3.

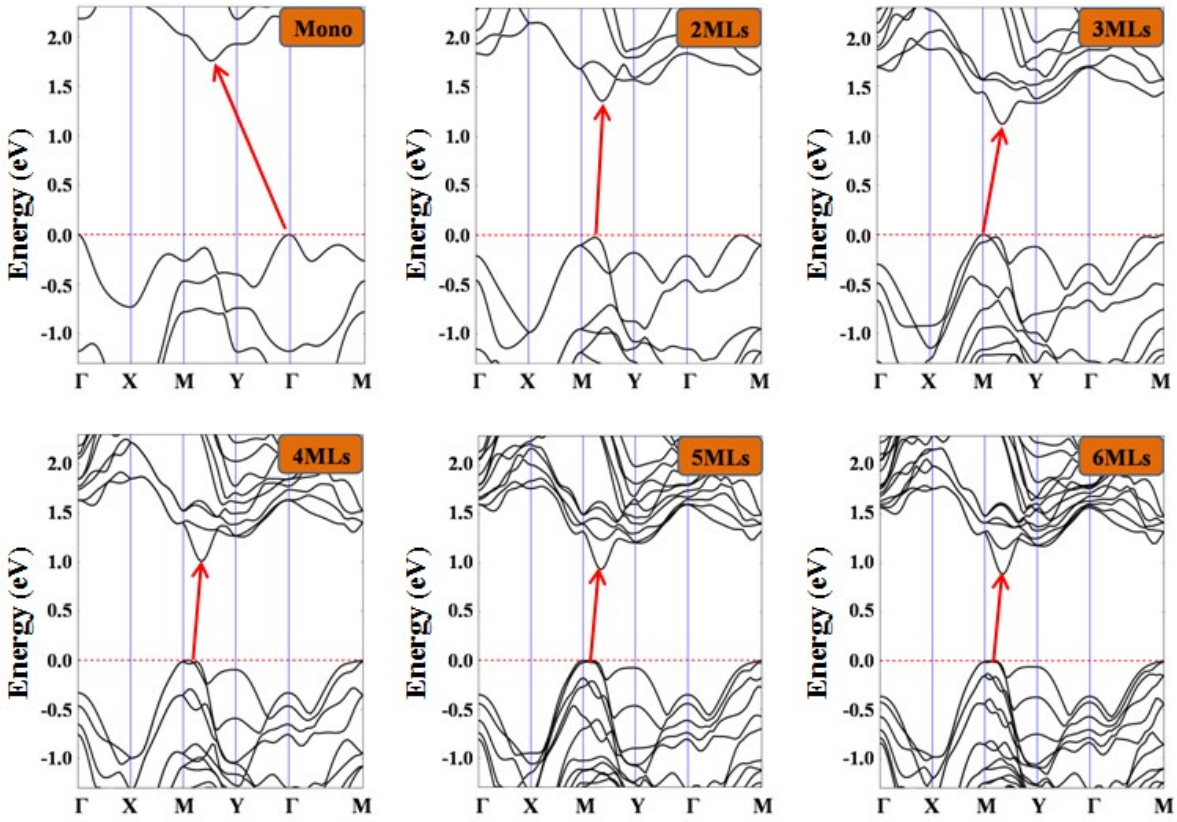

Figure S5. PBE band structures of α-Se from n=1 to n=6.

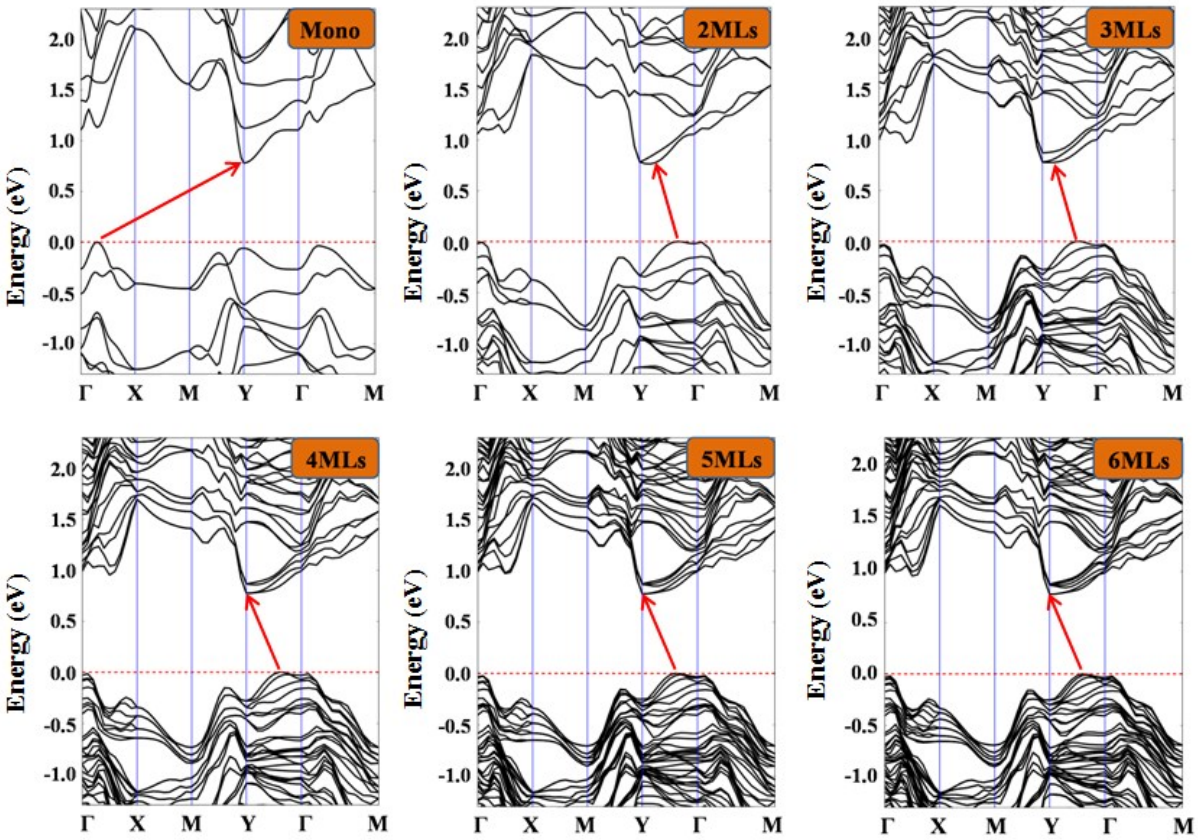

Figure S6. PBE band structures of Sb_2Se_3 from n=1 to n=6.

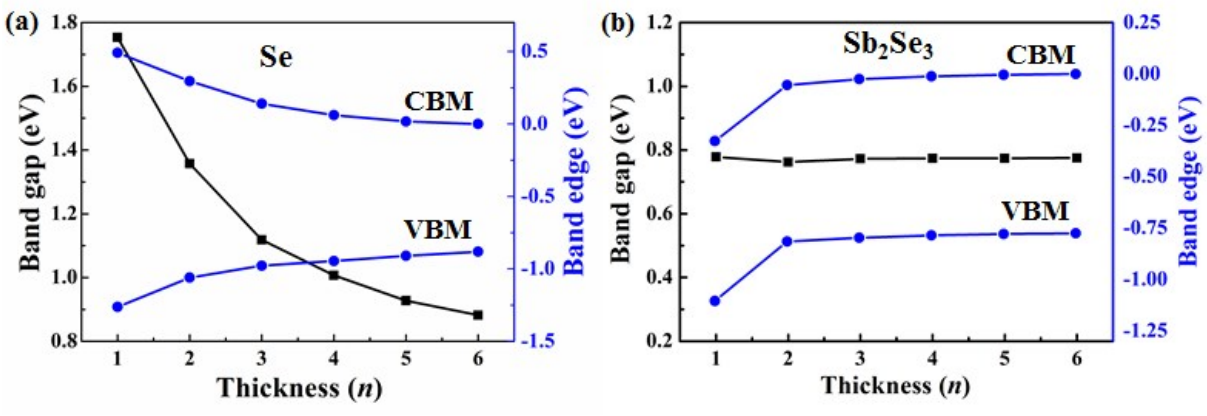

Figure S7. PBE band gaps and band edge evolution with layer number increases of few layers α-Se (a) and Sb_2Se_3 (b).

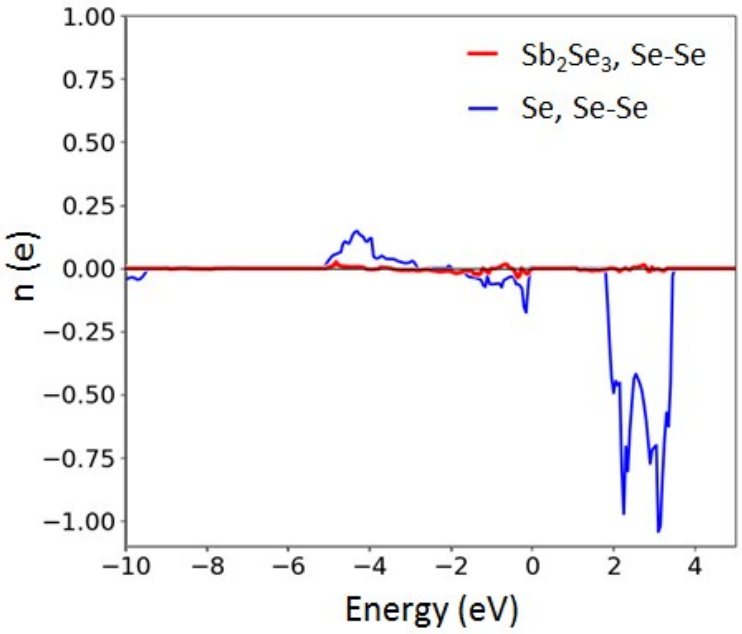

Figure S8. The crystal orbital Hamiltonian population (COHP) diagram of the Se-Se bonds in monolayer Se (blue line) and in Sb_2Se_3 (red line). The COHP adopts positive values to represent bonding interactions and negative values to identify antibonding interactions.

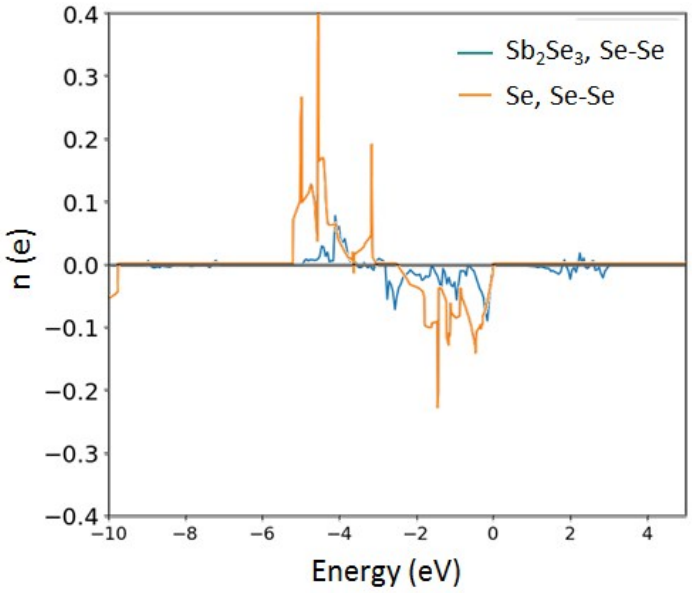

Figure S9 The crystal orbital Hamiltonian population (COHP) diagram of the Se-Se bonds in bilayer α-Se (orange line) and in Sb_2Se_3 (dark cyan line). The two Se atoms from each monolayer beside the interlayer region with the shortest Se-Se interlayer distance are selected for the bilayer COHP analysis.

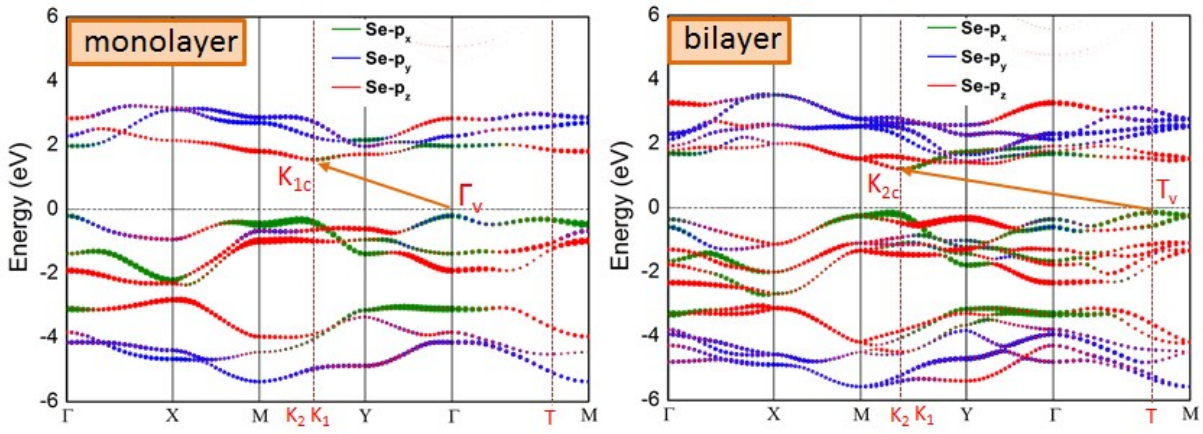

Figure S10. The projected HSE band structure of (a) monolayer and (b) bilayer α-Se.

The green, blue and red dot represent Se-px, py and pz orbits, respectively.

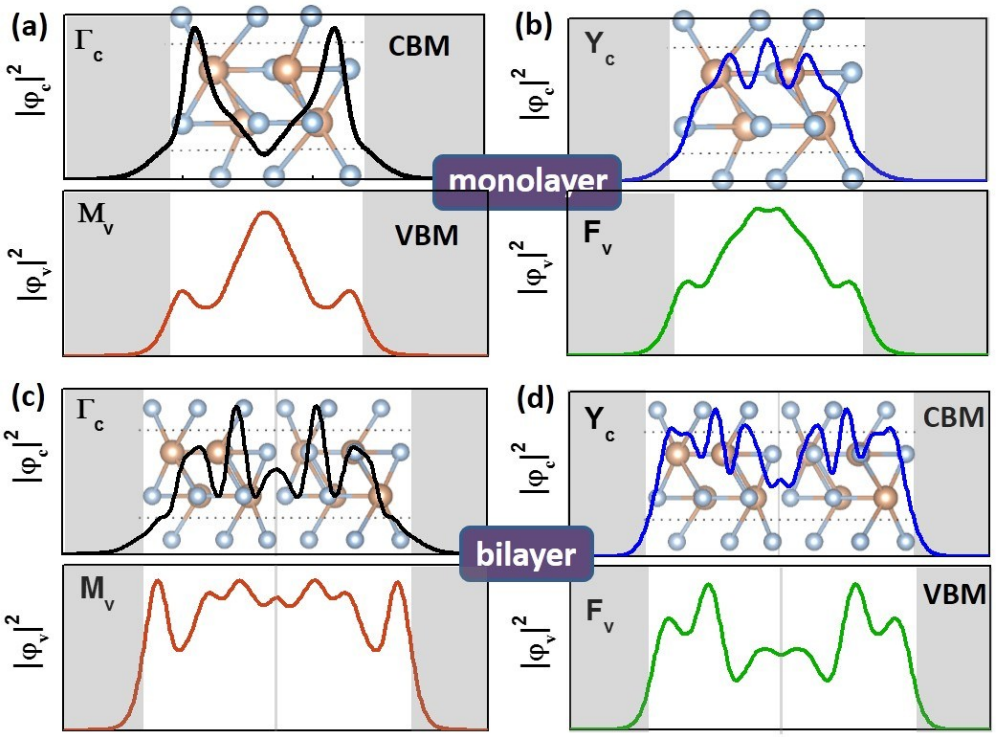

Figure S11 The planar-averaged squared wave function for top VB and top CB of monolayer and bilayer Sb_2Se_3. Γ and M represent the position in reciprocal space of the CBM of monolayer and bilayer Sb_2Se_3, Y and F represent the position in reciprocal space of the VBM of monolayer and bilayer Sb_2Se_3.

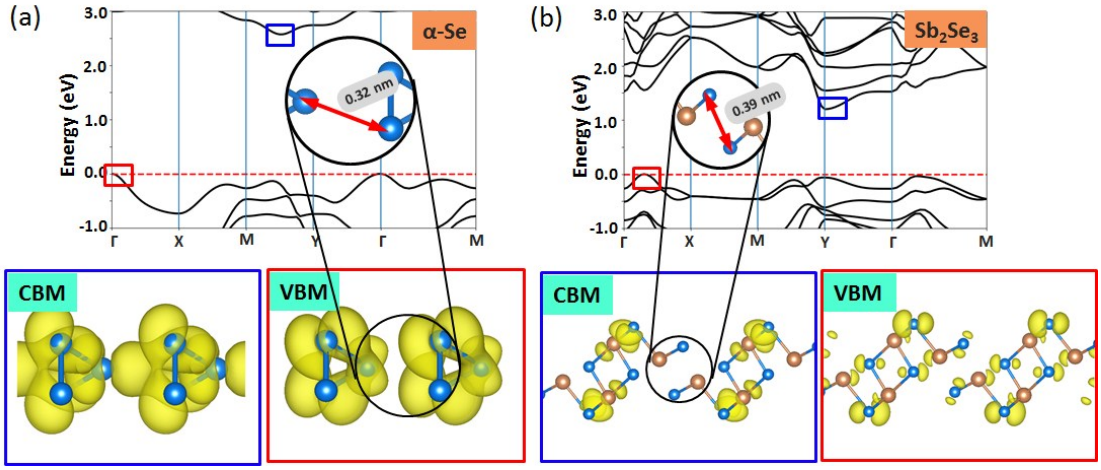

Figure S12. The visualized wavefunction of two chains structures of α-Se and Sb_2Se_3.