Supporting Information

Few-Layer Tin Sulfide: A New Black-Phosphorus-Analogure 2D Material with Sizeable Band Gap, Odd-Even Quantum Confinement Effect, and High Carrier Mobility

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Supporting Information Figures

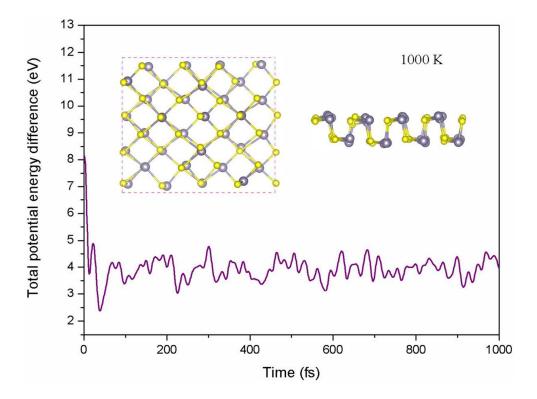


Figure SI1. Total potential energy fluctuation during AIMD simulations of monolayer SnS at 1000 K. The insets show the snapshot at 1ps for 4×4 supercell simulation.

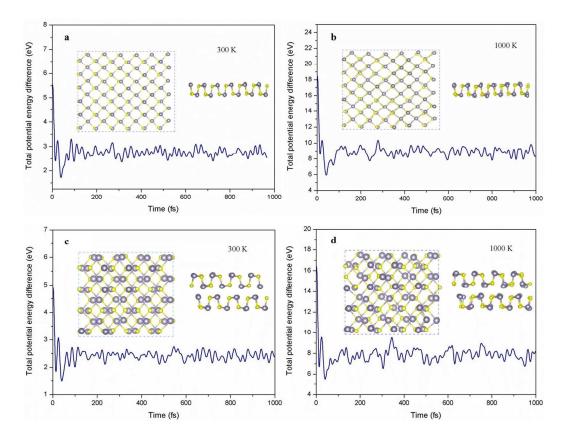


Figure SI2. Total potential energy fluctuation during AIMD simulations of SnS. (a,b) Monolayer at 300 K and 1000 K. (c,d) Bilayer at 300 K and 1000 K. The insets show the snapshot at 1ps for monolayer 6×6 and bilayer 4×4 supercell simulation.

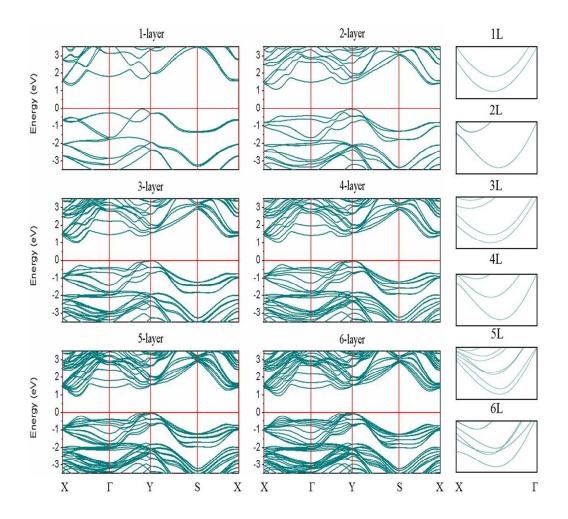


Figure SI3. Electronic band structures for bulk and few-layer (1-6) SnS. The magnified plotting of conduction-band minimum was placed at the right. Results were calculated using the PBE with SOC.

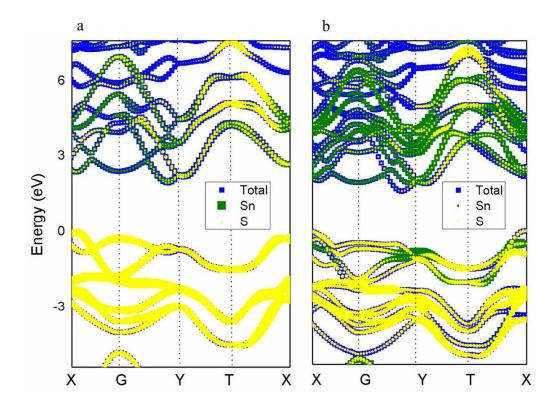


Figure SI4. Projection band structure of SnS. (a) monolayer, (b) bilayer.

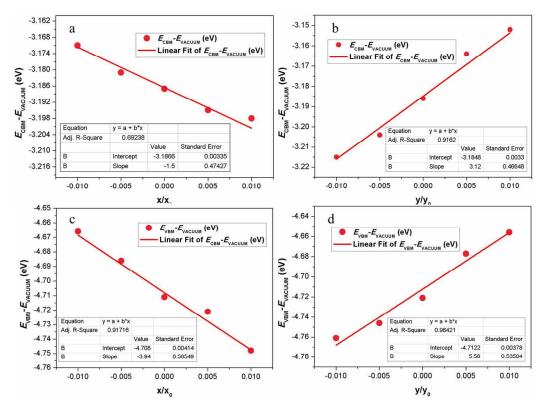


Figure SI5. Band energy of monolayer SnS. (a,b) The CBM of monolayer SnS. (c,d) The VBM of monolayer SnS.

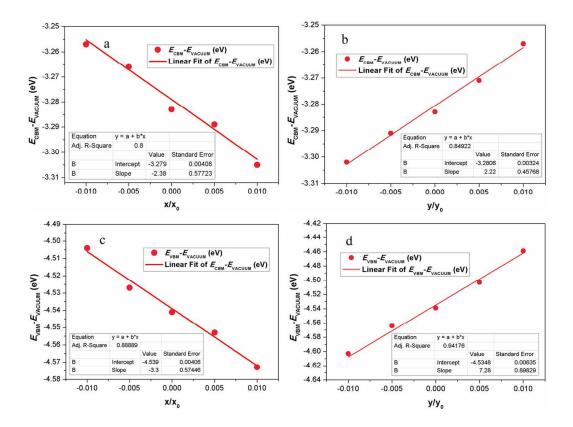


Figure SI6. Band energy of monolayer SnS. (a,b) The CBM of bilayer SnS. (c,d) The VBM of bilayer SnS.