

Supplementary Information

Interfacial Chalcogen Pair Mediated and Biaxial Strain Tuneable Type-2 Band Alignment in SnSSe Homogenous Bilayer- A Density Functional Theory-Based Analysis

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Structural and Electronic Properties of SnS₂, SnSe₂ and SnSSe Monolayer

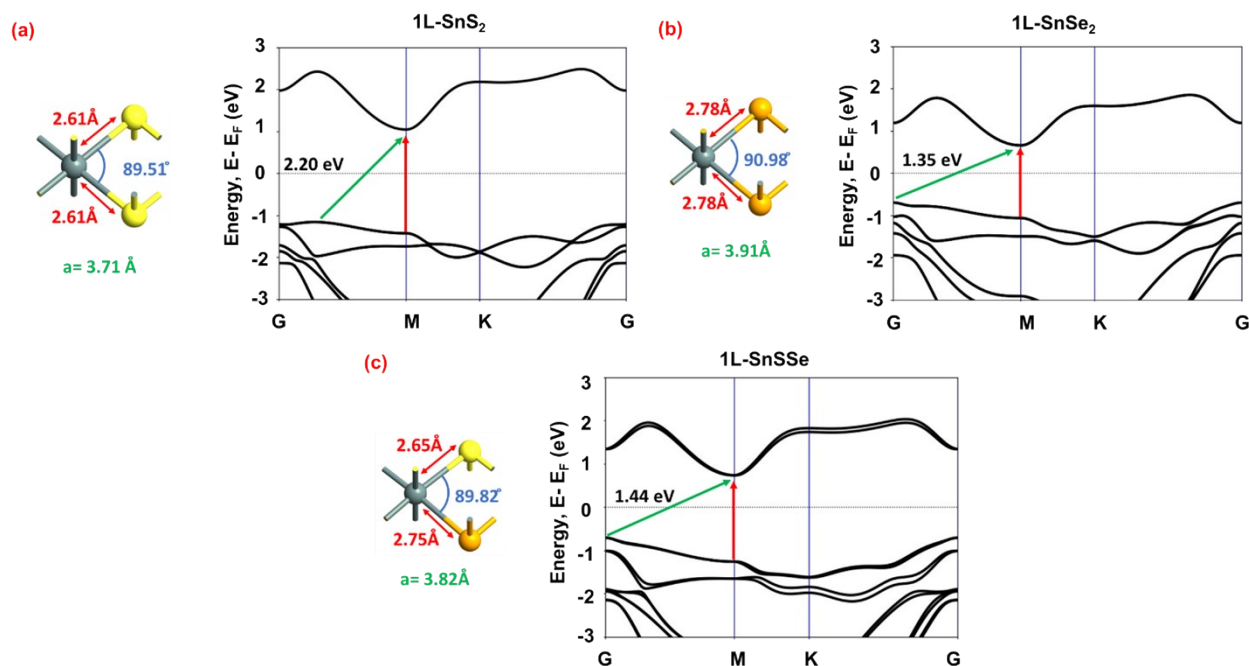
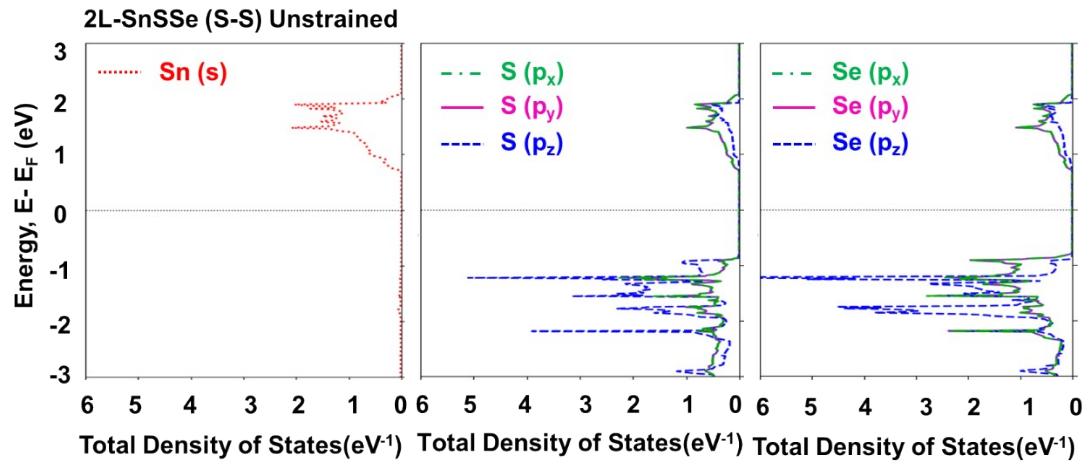


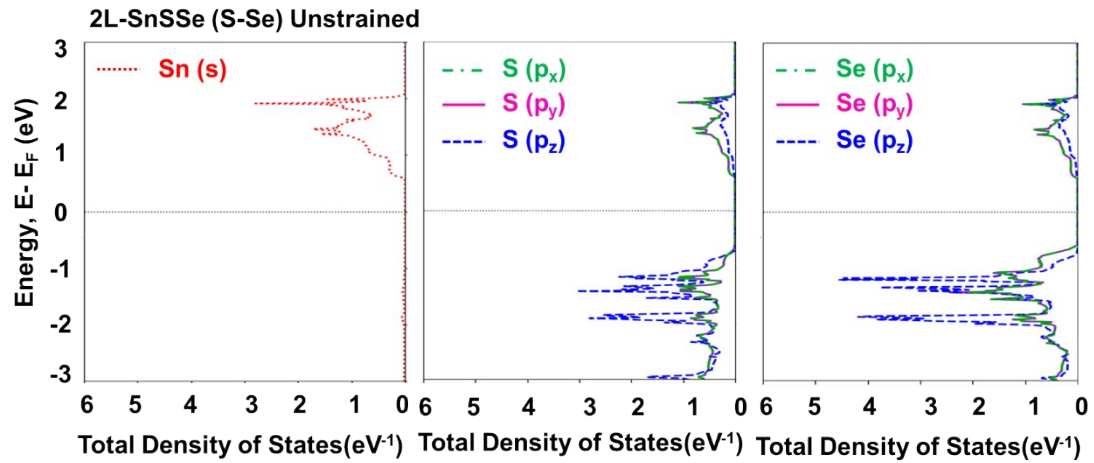
Figure S1. Structural and Electronic Properties of monolayers of (a) SnS₂ (b) SnSe₂ (c) SnSSe.

Influence of Interlayer Chalcogen Pairing on Atomic Orbital Projected Density of States (PDOS) of SnSSe Bilayers

(a)



(b)



(c)

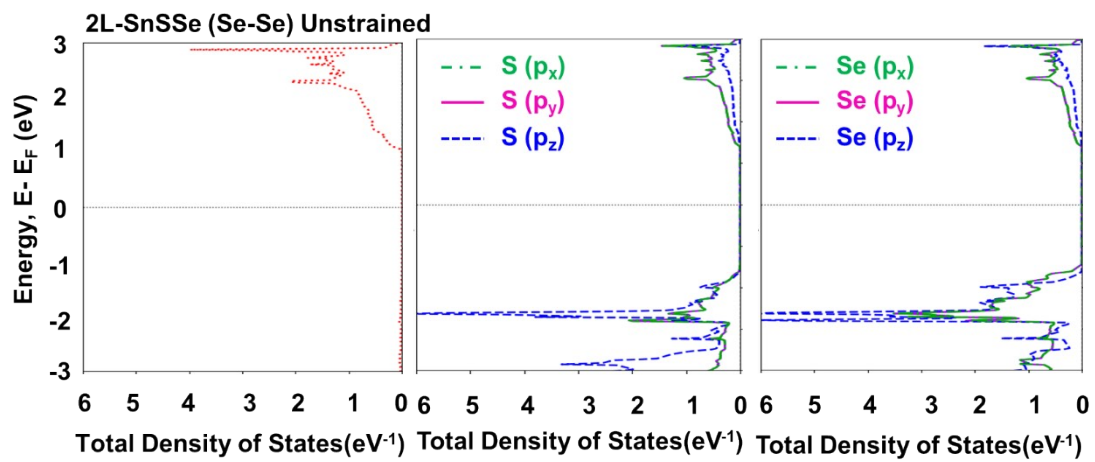
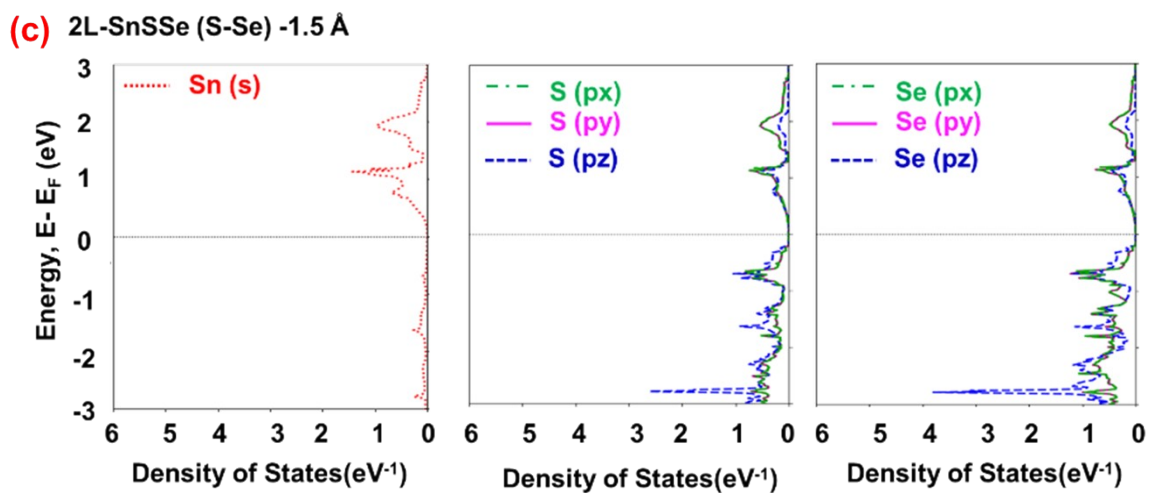
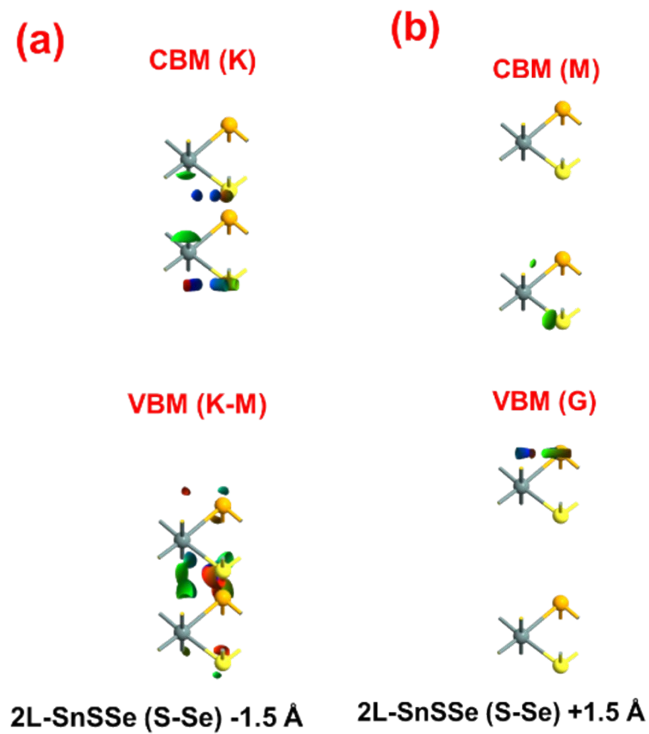


Figure S2. Individual atomic orbital projections on Projected density for SnSSe bilayers of (a) S-S (b) S-Se and (c) Se-Se chalcogen pair configurations.

Influence of Interlayer Distance Variations on Spatial Distribution of Bloch States, Total and Atomic Orbital Projected Density of States (PDOS) of SnSSe Bilayer in S-Se Configuration



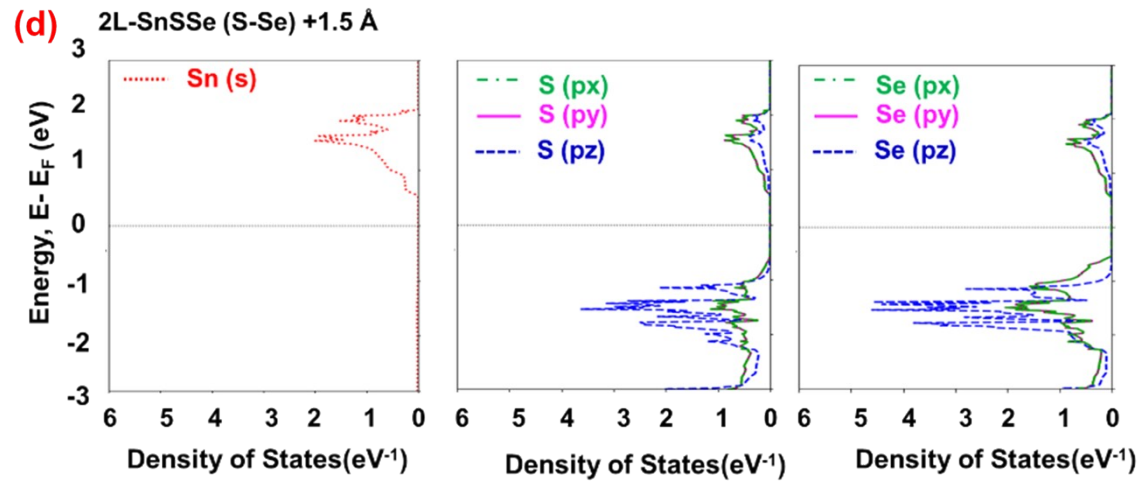


Figure S3. Plots of Bloch states for: (a) -1.5 Å and (b) 1.5 Å interlayer distance variations, plots of atomic orbital projected density of states for: (c) -1.5 Å (d) 1.5 Å interlayer distance variations in S-Se configuration of SnSSe bilayer.

Influence of Biaxial Strain on Structural Properties of SnSSe Bilayers in S-Se Interlayer Chalcogen Pair Configurations

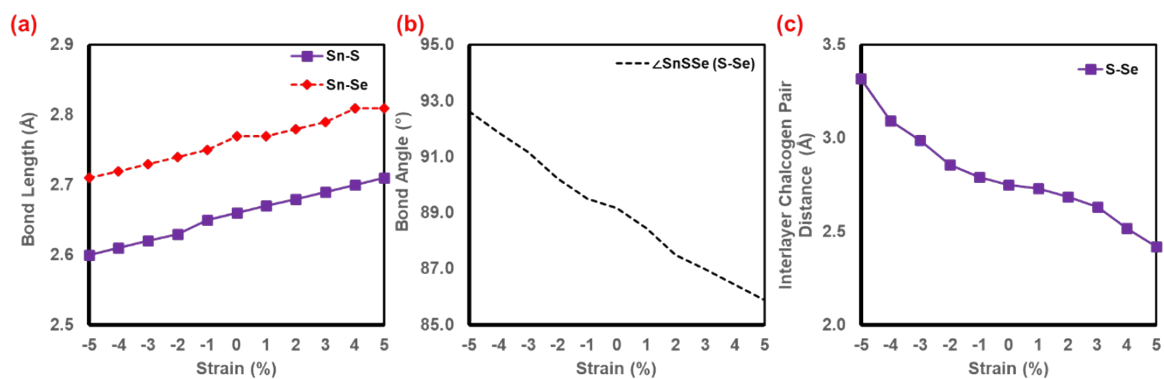
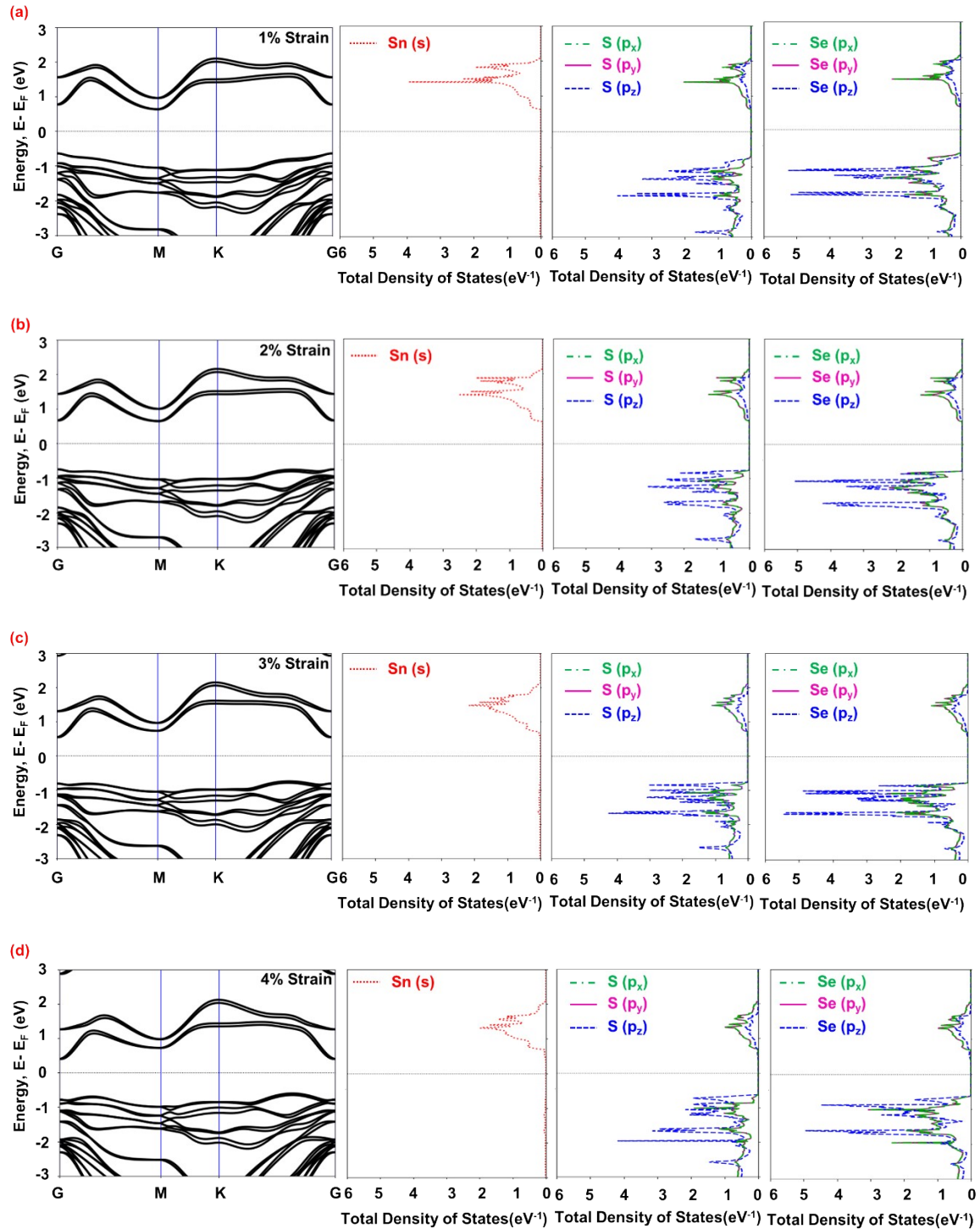


Figure S4. Plots of (a) bond length, (b) bond angle and (c) interlayer chalcogen pair distance as a function of strain for bilayer SnSSe in S-Se configuration.

Influence of Biaxial Strain on Band structures and Atomic Orbital Projected Density of States of SnSSe Bilayers in S-Se Interlayer Chalcogen Pair Configurations



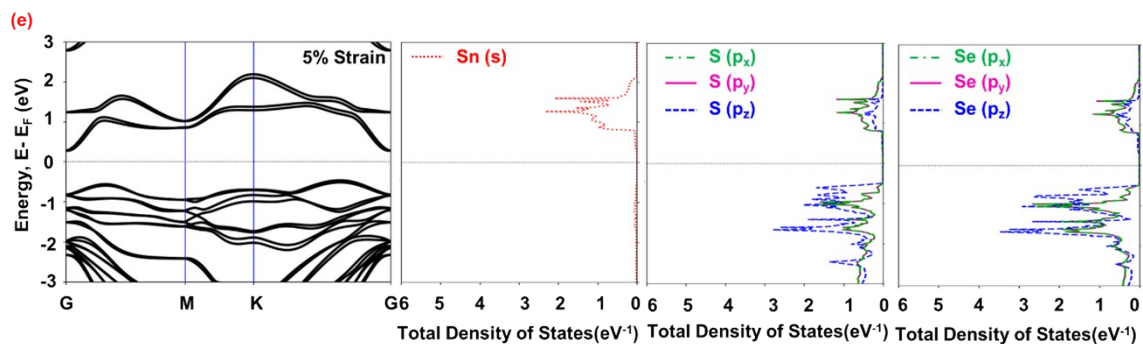
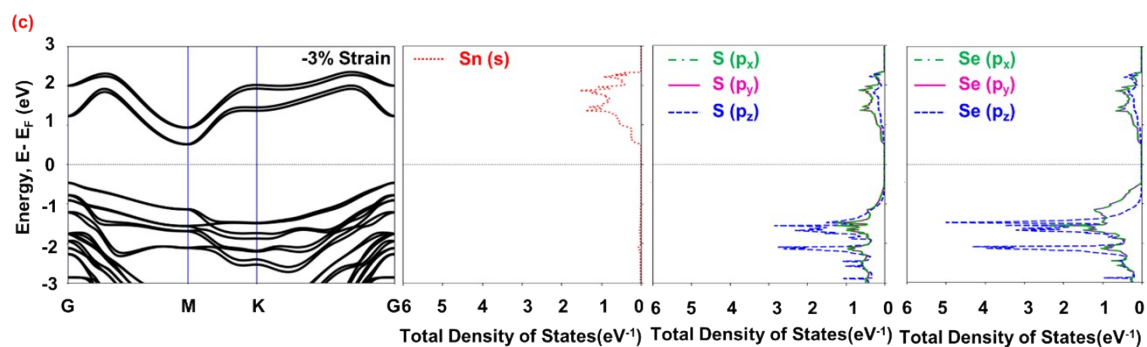
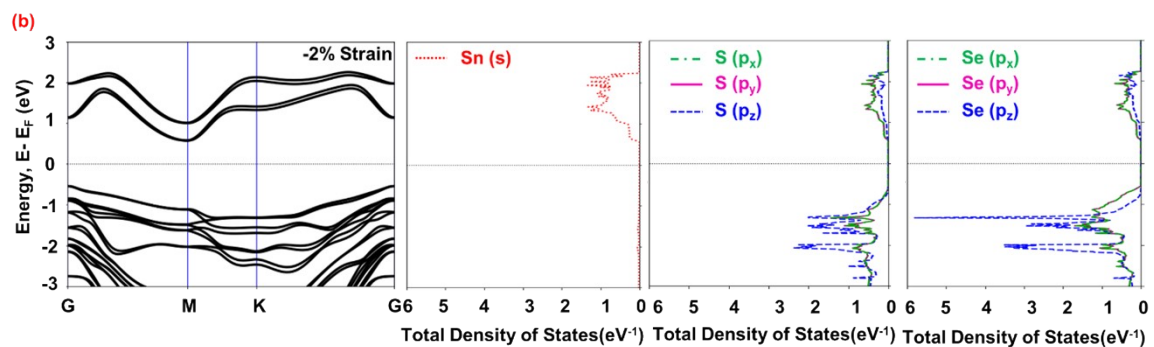
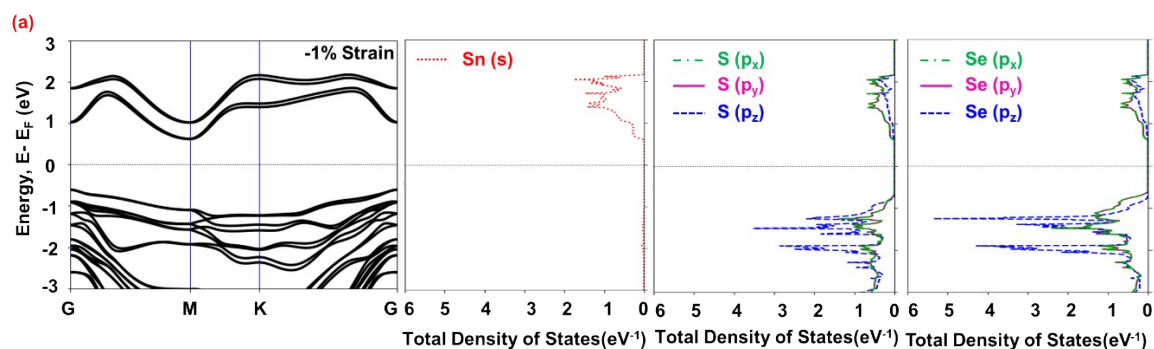


Figure S5. Plots of band structures and individual atomic projected density of states as a function of (a) 1%, (b) 2%, (c) 3%, (d) 4%, and (e) 5% BC strains for bilayer SnSSe of S-Se configurations.



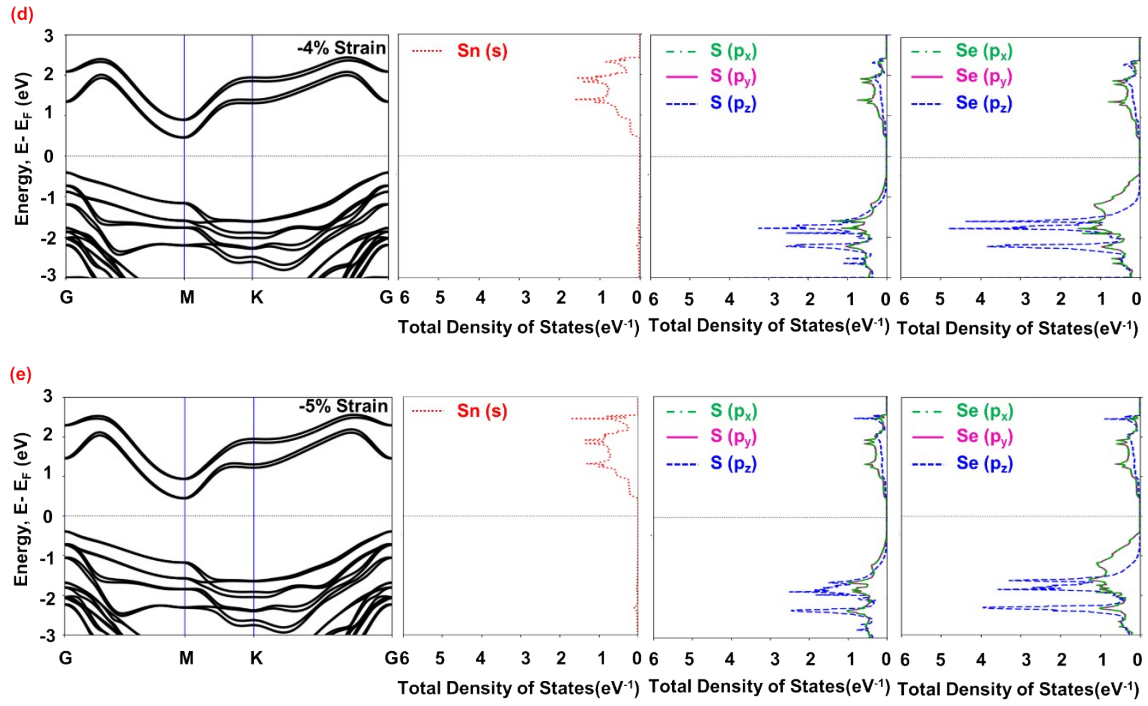


Figure S6. Plots of band structures and individual atomic projected density of states as a function of (a) -1%, (b) -2%, (c) -3%, (d) -4%, and (e) -5% BT strains for bilayer SnSSe of S-Se configurations.

Influence of Biaxial Strain and Interlayer Distances on Conduction Band Spread in Energy for SnSSe Bilayers in S-Se Interlayer Chalcogen Pair Configurations

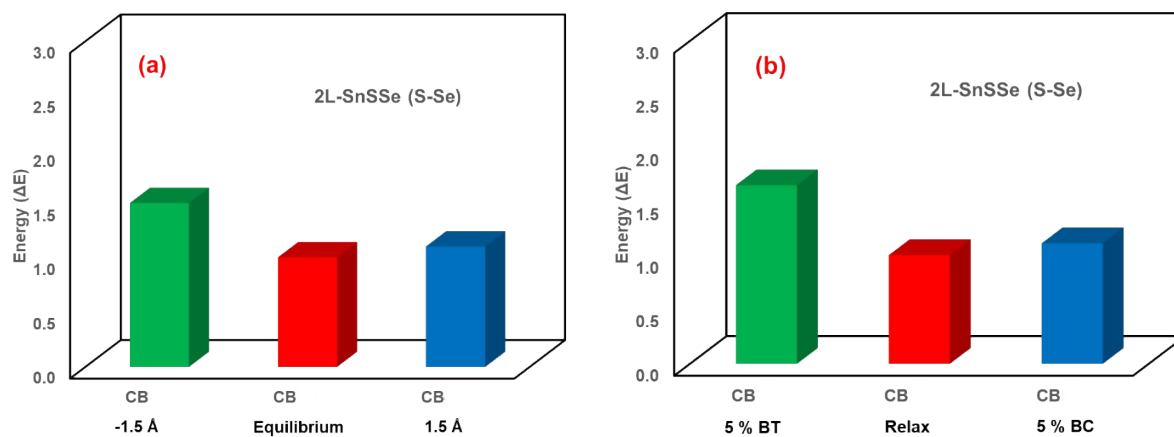


Figure S7. Plots of conduction band spread over energy for (a) different interlayer distance, and (b) different biaxial strain.