Electric Field and Uniaxial Strain Tunable Electronic Properties in InSb/InSe Heterostructure

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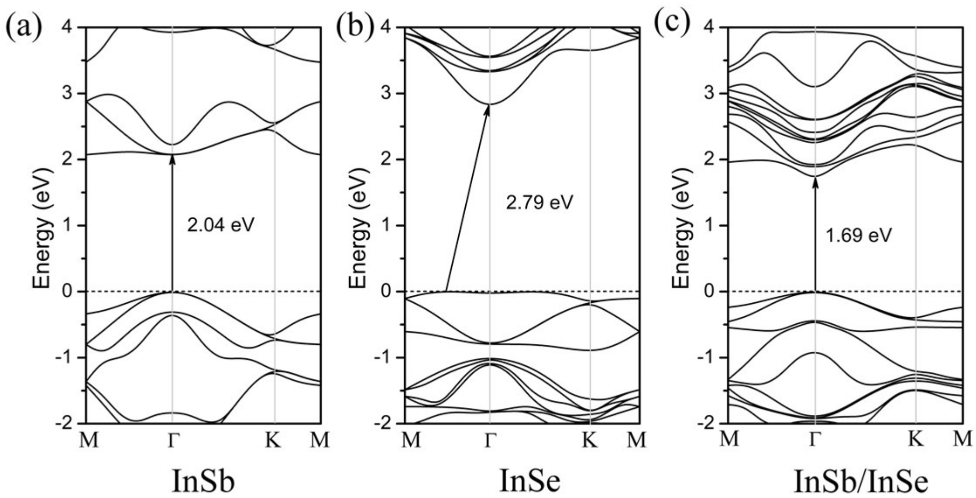

Fig. S1. Band structures of the InSb monolayer (a), InSe monolayer (b), and InSb/InSe heterostructure (c) calculated by HSE06, respectively.

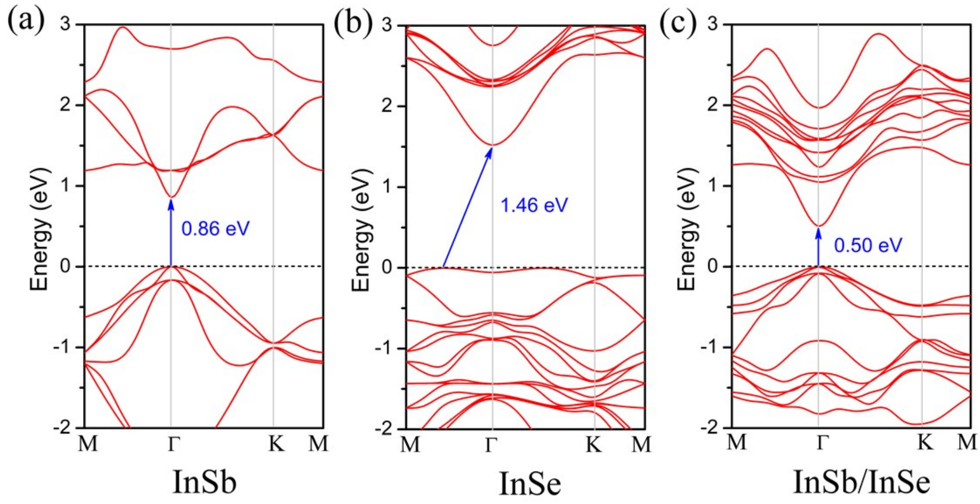

Fig. S2. (a-c) are the band structures of the freestanding InSb, InSe monolayer and InSb/InSe heterostructure with SOC, respectively.

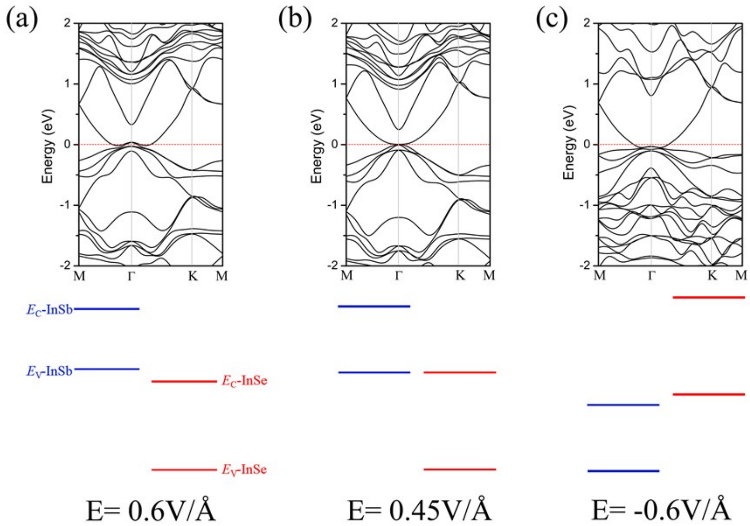

Fig. S3. The projected band structures (top) and corresponding band alignments (bottom) at E_{ext} = 0.6, 0.45, -0.6 V $Å^{-1}$, respectively.

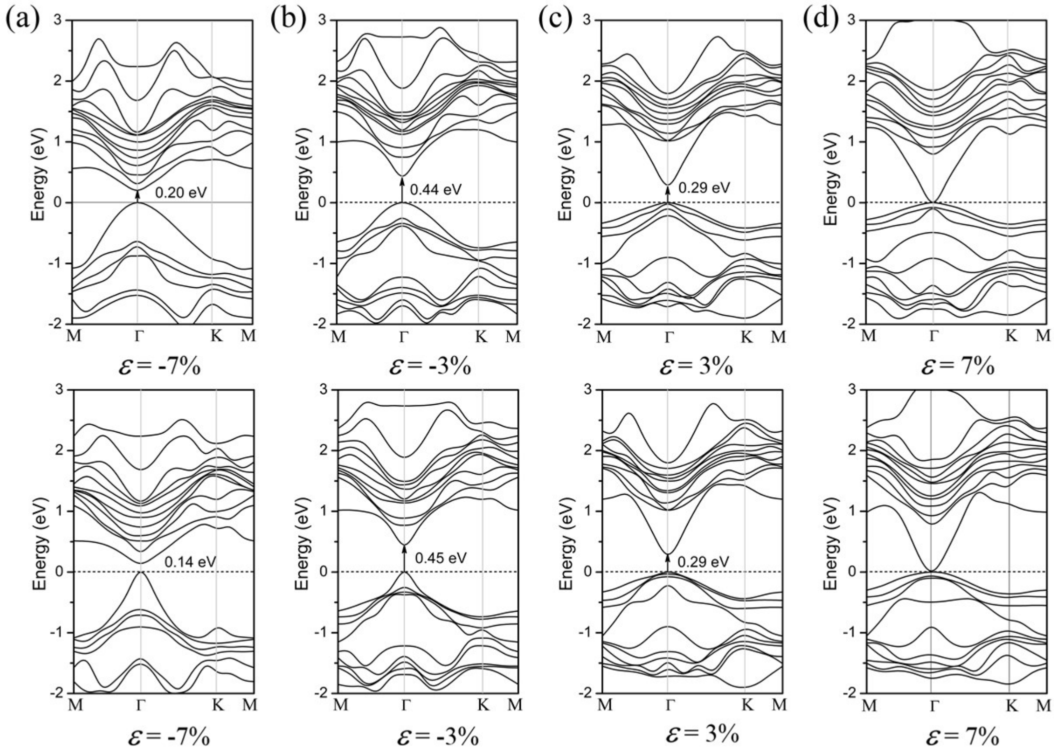

Fig. S4. Projected band structures of the InSb/InSe heterostructure under -7% (a), -3% (b), 3% (c), and 7% (d) strains, respectively. The upper part is under the X-axis strain and the lower part is under the Y-axis strain.

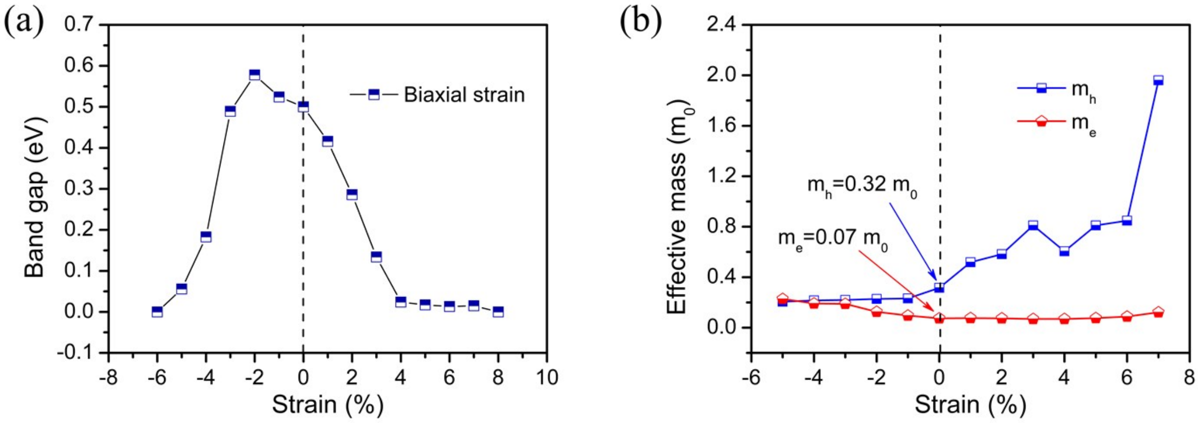

Fig. S5. (a) Variation trend of band gap with biaxial strain. (b) Effective mass of the heterostructure under biaxial strain.

From the results, it can be seen that the band gap decreases monotonically with increasing strain when tensile strain is applied. When the strain reaches 4%, as the strain continues to increase, the band gap changes only slightly. When the strain exceeds 8%, the band gap is suddenly closed. Conversely, when compressive strain is applied, the band gap increases with increasing strain in the range of 0 to 2%. After that, the band gap quickly decreases as the strain increases, until it is zero at 6%. Besides, the effect of biaxial strain on the effective mass of carriers is also discussed. It can be seen that the effective mass of holes increases significantly while the effective mass of electrons hardly changes as the strain increases under tensile strain. When compressive strain is applied, as the strain increases, the effective mass of holes decreases slightly, and the effective mass of electrons also increases slightly. Finally, the effective mass of electrons and holes reaches the same level under compressive strain.