# Supplementary Information

# Strain-engineered thermophysical properties ranging from band insulating to topological insulating phases in β-Antimonene

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## 1. Crystal Orbital Hamiltonian Population (COHP)

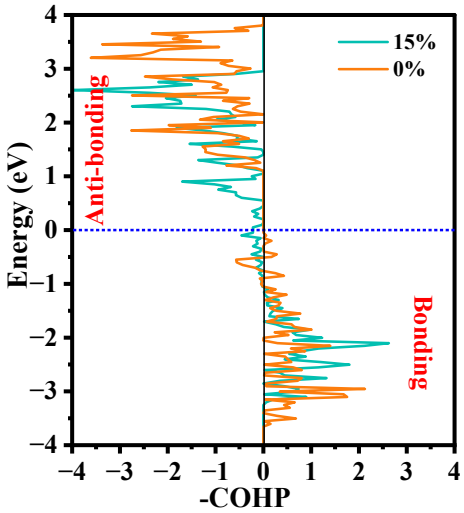


**Fig. S1:** The Crystal Orbital Hamiltonian Population comparing (-COHP) for 0% to 15 % strain. Near fermi level the relatively larger population of the antibonding states at 15% strain indicate the weaking in covalent bond leading a anharmonicity.

## 2. Mechanical & Structural Properties:

**Table S1:** Elastic stiffness Coefficients, bulk modulus (B), density ($\rho$), the sound velocity in transverse ($v_t$) and longitudinal direction ($v_l$) for the pristine and strained β-Sb system.

| Strain | $C_{11}$ (N m$^{-1}$) | $C_{12}$ (N m$^{-1}$) | $C_{66}$ (N m$^{-1}$) | B (N m$^{-1}$) | $\rho$ (kg m$^{-2}$) | Poisson ratio | $v_t$ (km s$^{-1}$) | $v_l$ (km s$^{-1}$) |
|---|---|---|---|---|---|---|---|---|
| 0% | 32.746 | 6.395 | 13.176 | 19.571 | $2.75 \times 10^{-6}$ | 0.195 | 2.18 | 3.45 |
| 5% | 23.761 | 5.619 | 9.071 | 14.690 | $2.54 \times 10^{-6}$ | 0.236 | 1.90 | 3.09 |
| 10% | 17.018 | 4.234 | 6.392 | 10.626 | $2.27 \times 10^{-6}$ | 0.248 | 1.68 | 2.74 |
| 15% | 6.259 | 1.099 | 2.580 | 3.679 | $2.08 \times 10^{-6}$ | 0.176 | 1.13 | 1.73 |

The average sound velocity in the crystal is given by;

$$v_s = \left[\frac{1}{3}\left(\frac{1}{v_l^3} + \frac{2}{v_t^3}\right)\right]^{-\frac{1}{3}} \#(1)$$

Where $v_l$ and $v_s$ are the longitudinal and transverse sound velocity and given as follows;

$$v_l = \left(\frac{B+G}{\rho_{2D}}\right)^{\frac{1}{2}} \#(2)$$

$$v_t = \left(\frac{G}{\rho_{2D}}\right)^{\frac{1}{2}} \#(3)$$

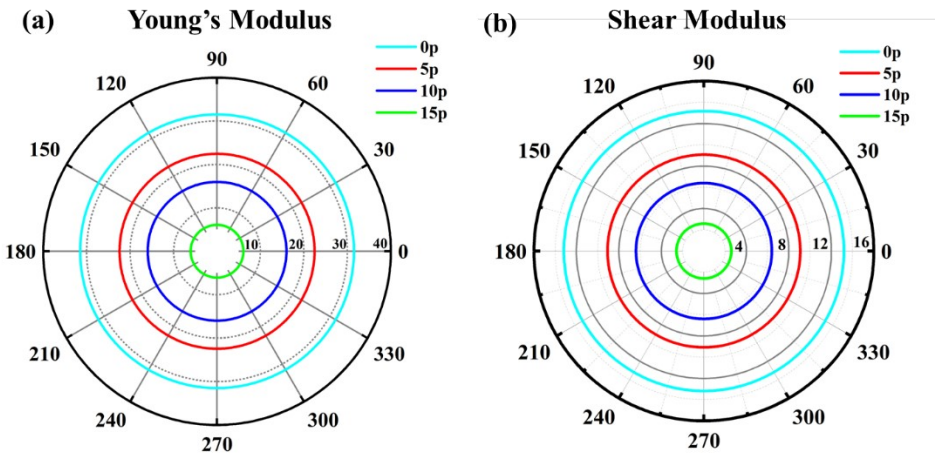


**Fig. S2**: The isotropic Young's Modulus (Y) and Shear Modulus (G) for the range of strain 0% to15 %. A reduction in its value indicates the reduction in bond strength with increasing biaxial strain.

**3. Biaxial strain effect on Bandgap:**

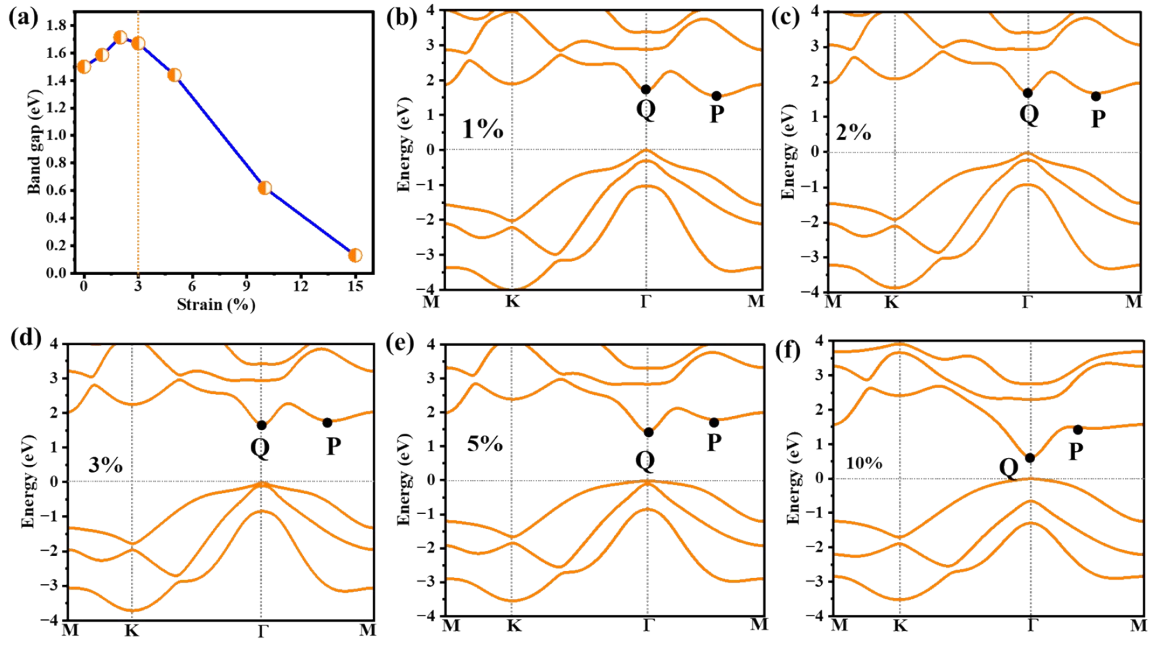


**Fig. S3**: Biaxial strain effect on the bandgap value (HSE06) for the range of strain 0% to 15 % in β-Sb monolayer. The dotted vertical line shows indirect to direct bandgap transition at ~ 3% strain (b-f) Calculated HSE06, the electronic band structure of β-Sb including SOC for different strain (b) 1% strain (c) 2% strain (d) 3% strain (e) 5% strain (f) 10% strain.

**4. Z2 Invariant in topological insulator:**

In two-dimensions, to distinguish the quantum spin Hall phase from the band insulator, the $Z_2$ invariant is defined. Following Fu et al. approach, $Z_2$ invariant can also be determined in the presence of inversion symmetry, through parity of the occupied band eigenstates at the four time-reversal invariant momenta (TRIM) $\Gamma_i$ points. This can be given by the quantities.

$$\delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i) \#(4)$$

Where, $\xi_{2m}(\Gamma_i) = \pm 1$ is the parity eigenvalue of the 2m$^{th}$ occupied energy band at $\Gamma_i$. The $Z_2$ invariant $= 0,1$ which determine the quantum spin-Hall phase, and is given as the product of $\delta_i$'s.

$$(-1)^{v} = \prod_{i} \delta_i \#(5)$$

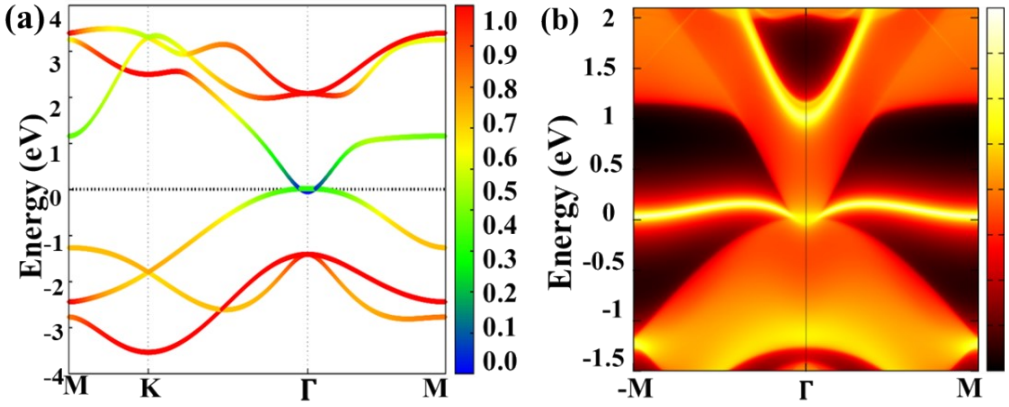


**Fig. S4:** (a) HSE06 based (without considering spin-orbit coupling) orbital projected band structure of β-Sb monolayer at 15% strain when no spin-orbit coupling is considered. The red colour denotes the complete p-orbital contribution. The dotted line indicates the fermi level. (b) Surface DOS for the 15% case within -1.5 eV to 2 eV energy range. The bright yellow region near fermi level signifies the two branches of overlapped edge states.

**5. Weighted Phase space of phonon-phonon scattering:**

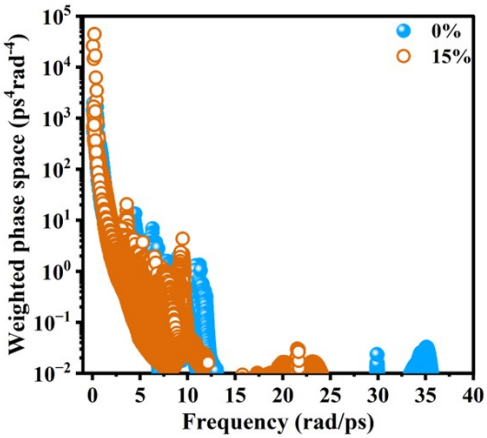


**Fig. S5:** Weighted phase space vs frequency (rad/ps) curve for 0% and 15% tensile strain.

**6. Mild Strain Raman Spectra**

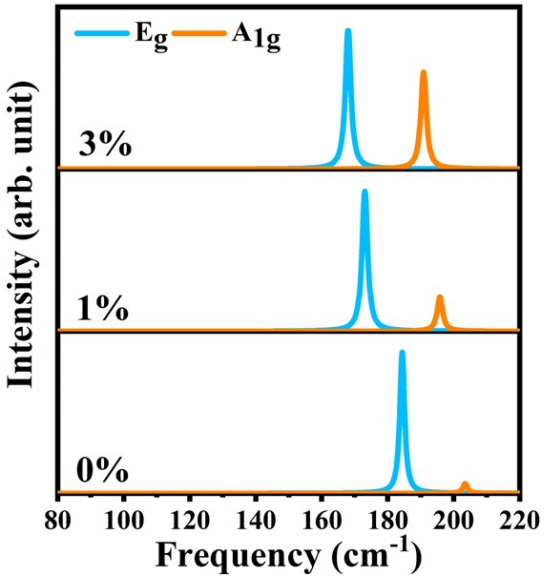


**Fig. S6:** Calculated Raman spectra as a function of frequency ($cm^{-1}$), under mild tensile strain ranging 0%, 1% and 3%. Orange and blue peaks represent the $A_{1g}$ and $E_g$ modes, respectively.