Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Tunable electronic properties of Sb/InSe van der Waal heterostructure by electric field effects

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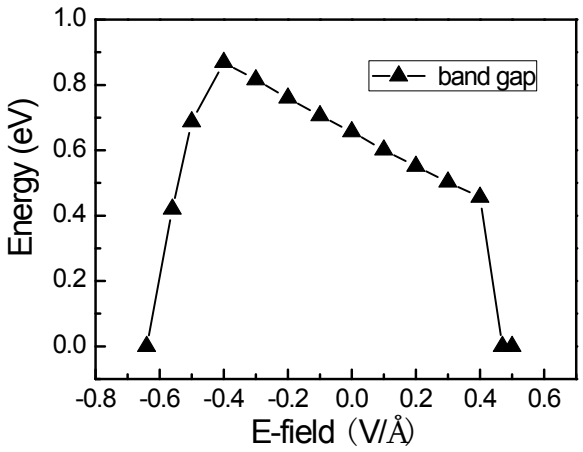

Figure S1. The evolution of the band gap of type H4 as a function of the E_{ext} in the Sb/InSe heterostructure.

Increasing the intensity of the positive E_{ext} leads to a decrease in the band gap until it disappears under an electric field that does not exceed 0.5 V/Å. However, the band gap increases first then rises to a maximum of 0.869 eV and finally falls to zero when a negative E_{ext} of 0.64 V/Å is applied. In the process of altering the applied E_{ext} from -0.64 to 0.5 V/Å, we observe that the band structure of type H4 always maintains a direct band gap with CBM and VBM remain at the Γ-point all the time. Compared with structure H3, the band gap of type H4 shows a similar trend by applying a perpendicular electric field.

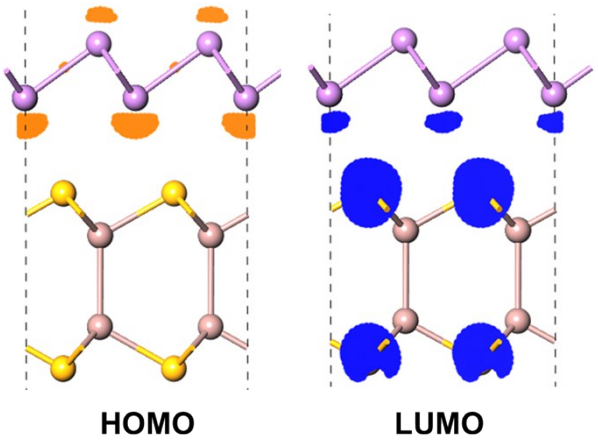

Figure. S2. Lowest unoccupied molecular orbitals (blue part) and highest occupied molecular orbital (orange part) isosurface of Sb/InSe heterostructure.

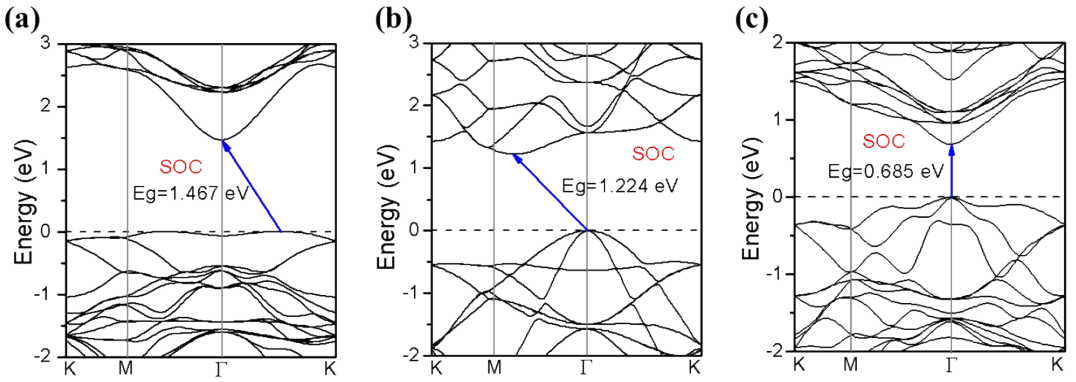

Figure. S3. (a)-(c) Band structures of monolayer InSe, monolayer Sb and Sb/InSe heterostructure in the presence of SOC effect, respectively. The Fermi level is shown by a black dashed line.

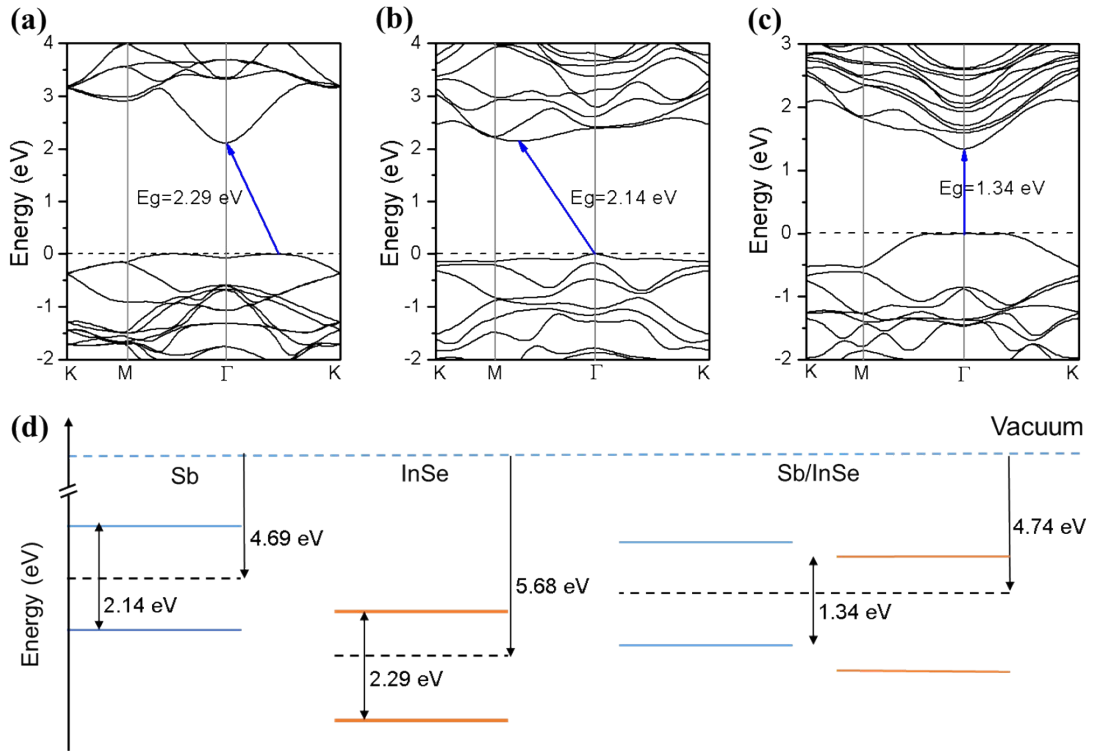

Figure S4. (a)-(c) Band structures of monolayer InSe, monolayer Sb and Sb/InSe heterostructure under HSE06 level, respectively. The Fermi level is set as zero. (d) Band alignments of monolayer Sb, monolayer InSe and Sb/InSe heterostructure. Relevant electronic parameters are also given in the Figure. The black dashed lines are the Fermi level. The vacuum level is taken as a reference.

The carrier effective mass can be calculated by the following equation:

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{h^2}\frac{\partial^2 E}{\partial k_i \partial k_j}, i, j = x, y, z \tag{1}$$

From the Equation, we can obtain the effective mass of the electron (or hole) by the second derivative of the top of the valence band (or the bottom of conduction band) for the wave vector. Although m^* is a second-order tensor with nine components, we can take it as a scalar. Three directions (*x, y, z*) are calculated when we calculate energy band.

$$\frac{1}{m^*} = \frac{1}{h^2}\frac{\partial^2 E(k)}{\partial k^2} \tag{2}$$

where k is the wave vector, $\hbar$ is the reduced Planck constant, and $E(k)$ is the dispersion relation.

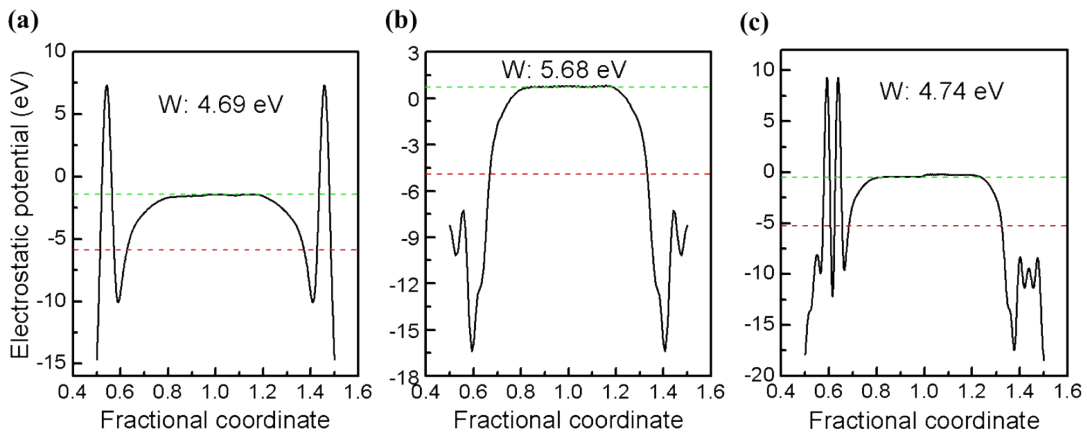

Figure. S5. Computed work function values for monolayer Sb (a), monolayer InSe (b) and Sb/InSe heterostructure interface (c), respectively. Red dashed lines represent the Fermi levels. Green dashed lines represent the vacuum levels.