Electronic Supplementary Material (ESI) for CrystEngComm.

Theoretical design of photodetector based on two-dimensional Sb/AlAs type-II heterostructure

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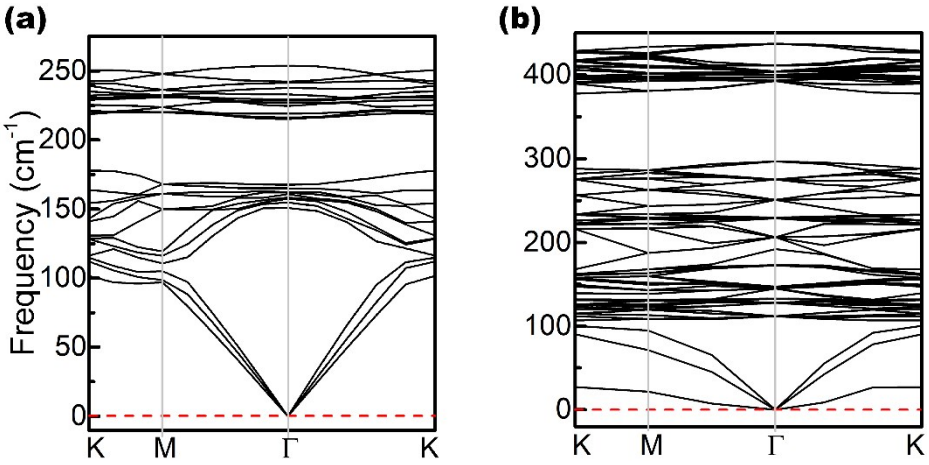

Fig. S1 The phonon dispersion curves of (a) Sb and (b) AlAs, respectively.

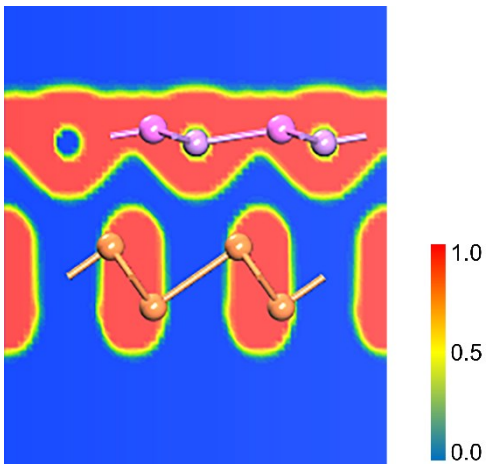

Fig. S2 Electron localization function (ELF) of the Sb/AlAs heterostructure. Red (blue) regions correspond to large (small) ELF values.

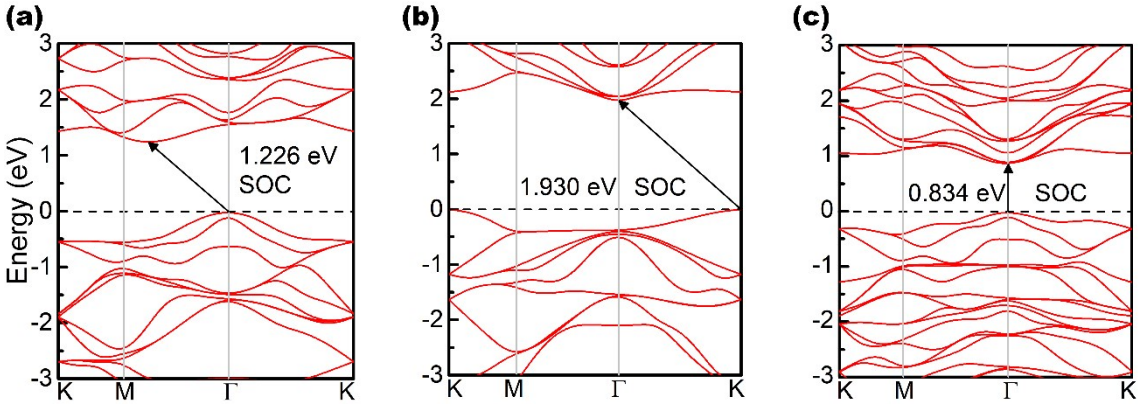

Fig. S3 The calculated band structures of (a) monolayer Sb, (b) AlAs and (c) Sb/AlAs heterostructure by SOC effect. The Fermi energy (E_F) is set as zero.

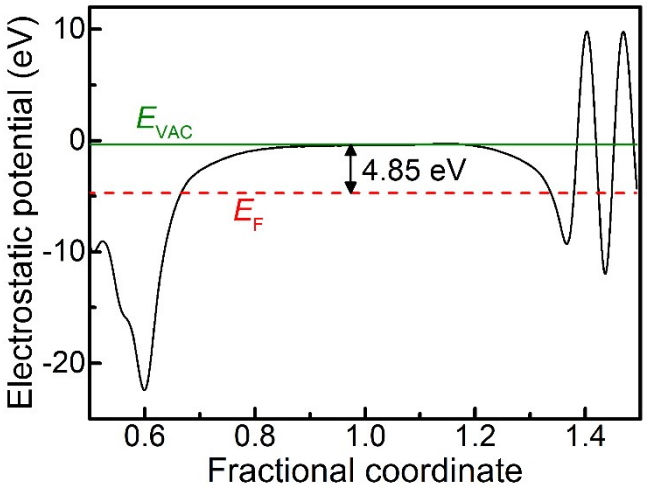

Fig. S4 The average electrostatic potential for Sb/AlAs heterostructure.

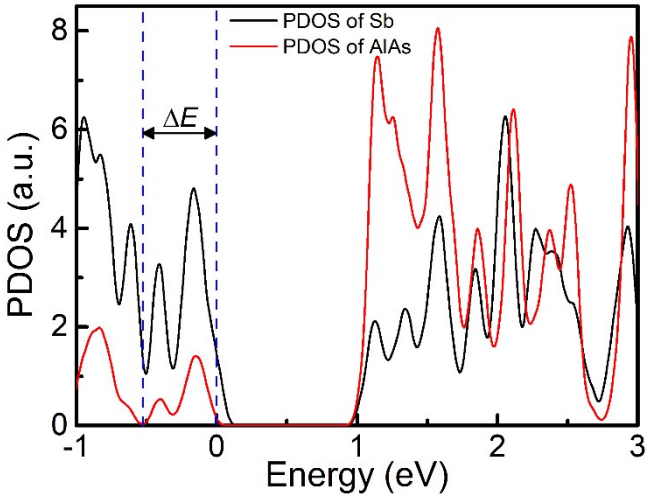

Fig. S5 PDOS method to obtain the band offset for Sb/AlAs heterostructure. The ΔE is the VBO.

We use the partial density of states (PDOS) method to obtain the band offset. We first perform DOS calculations on the Sb/AlAs heterostructure, and then select the Sb and Al atoms that relatively far from the interface (with less interface interaction) to obtain PDOS. This is because the vacuum levels of the materials on both sides of the interface in the heterostructure are aligned under equilibrium, so the energy difference between the VBM of Sb and AlAs is the VBO at the interface. Then use the equation of $\mathrm{CBO} = E_{g1} - E_{g2} - \mathrm{VBO}$ to obtain the CBO.

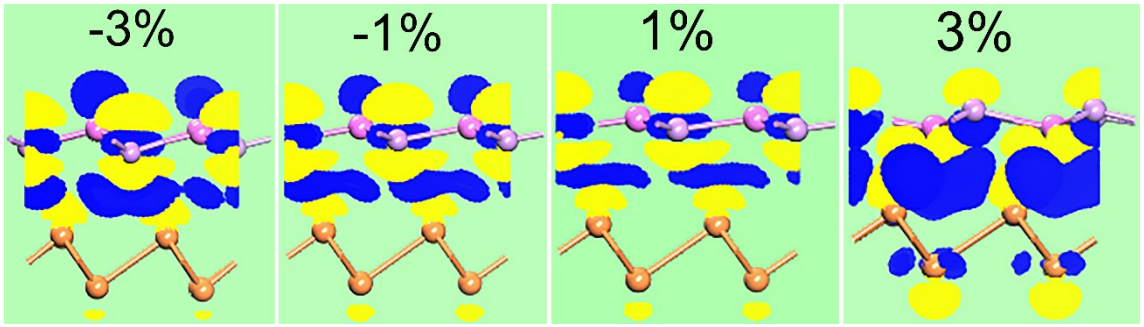

Fig. S6 The 3D plot of the charge density difference for the Sb/AlAs heterostructure under several representative biaxial strains. (According to the yellow isosurface, it can be seen that the number of charge transfer at the interface increases with the biaxial strain increases.)