# Supporting Information

## Biaxial strain effect on electronic structures tuning in antimonene-based van der Waals heterostructures

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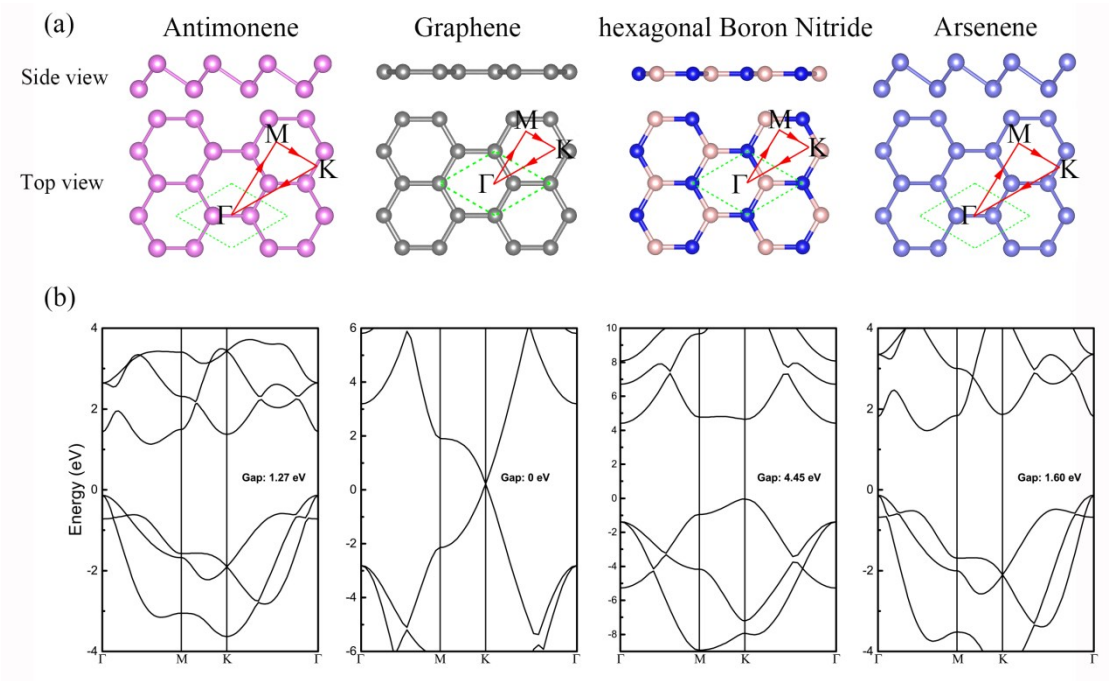


**Figure. S1.** (a) The side view and top view of antimonene, graphene, h-BN and arsenene monolayers atomic structures. Brilloun zone and specific symmetry points are listed on the top viewed monolayers atomic structures. (b) The calculated band structures with the PBE functional.

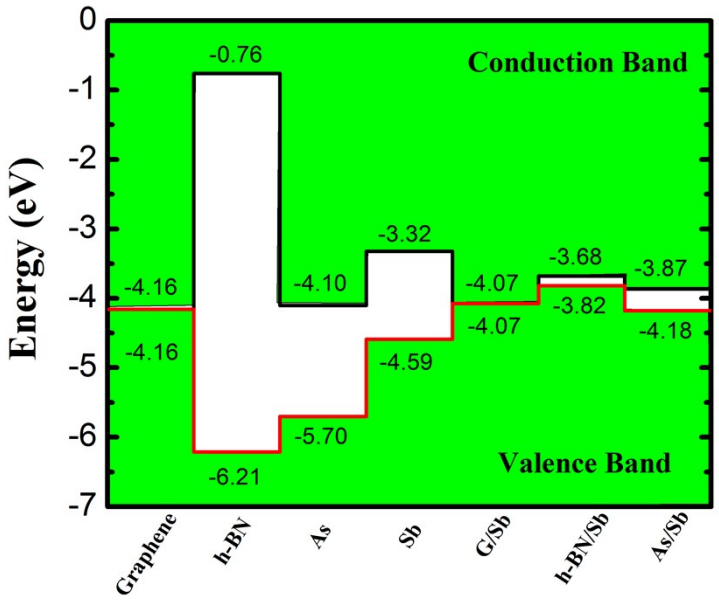


**Figure. S2** Calculated band alignment for results of the CBMs (VBMs) positions for the graphene, h-BN, arsenene, antimonene, and the corresponding antimonene-based heterostructures: G/Sb, h-BN/Sb, and As/Sb. The vacuum level is taken as zero reference.

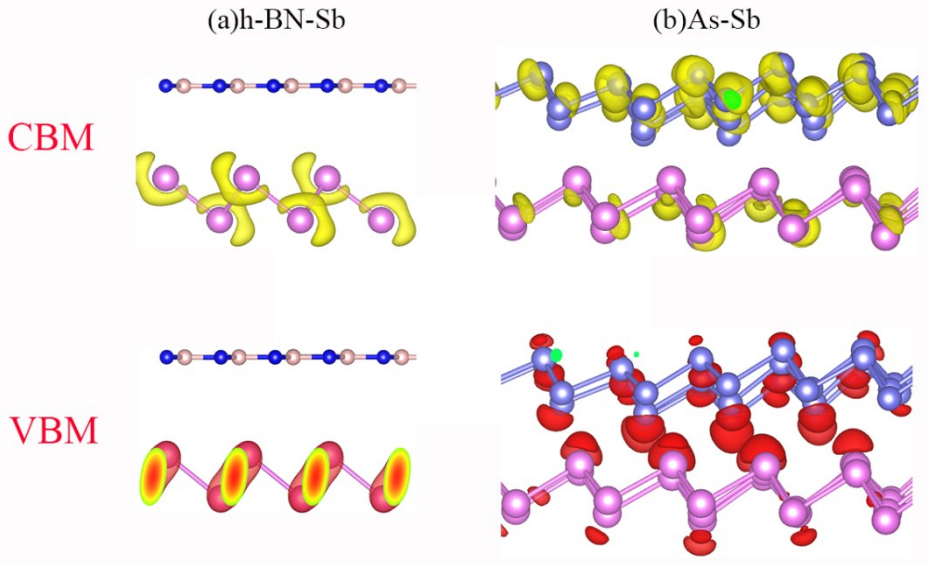


**Figure. S3** The corresponding charge densities of vdW heterostructures are shown in (a) h-BN-Sb (b) As-Sb (the isosurface values are 0.0035e/Å$^{-3}$, and 0.00085e/Å$^{-3}$ respectively). The CBMs in red isosurfaces (upper panel), and the VBMs in yellow isosurfaces (lower panel).

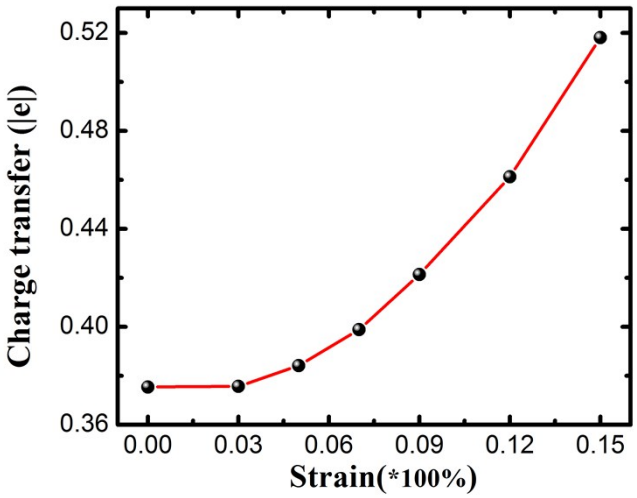


**Figure. S4** The amount of charge transfer of G/Sb heterostructures under biaxial strain of 0%-20%.

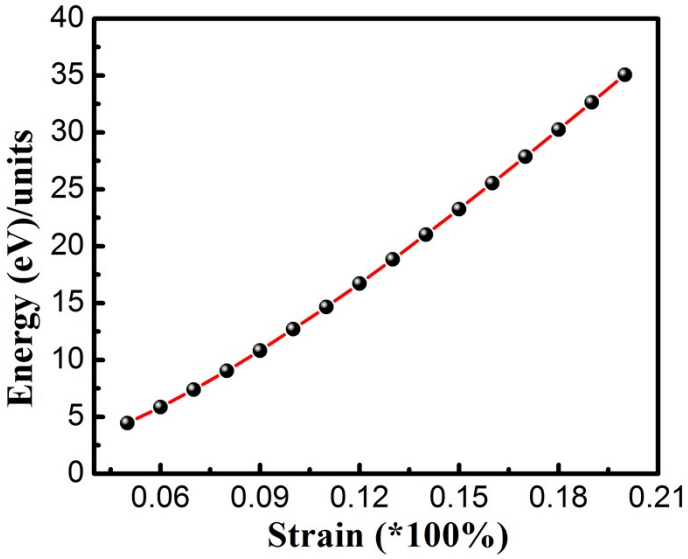


**Figure. S5** The energy difference between h-BN/Sb heterostructures under biaxial strain of 0%-20%.