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

Supplementary Information for Monolayer $Bi_2Se_{3-x}Te_x$: novel two-dimensional semiconductors with excellent stability and high electron mobility

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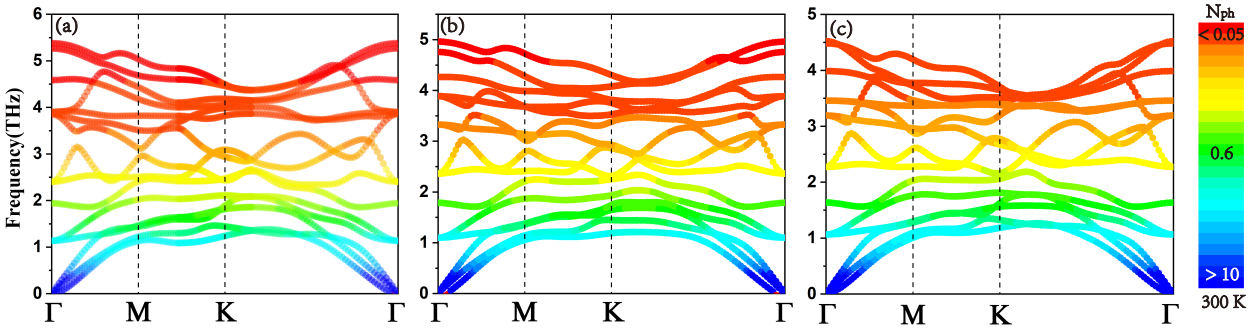

FIG. S1: Phonon dispersion of monolayer (a) Bi_2Se_3, (b) Bi_2Se_2Te and (c) Bi_2SeTe_2, respectively. The phonon occupation number is determined from the Bose-Einstein distribution function at 300 K.

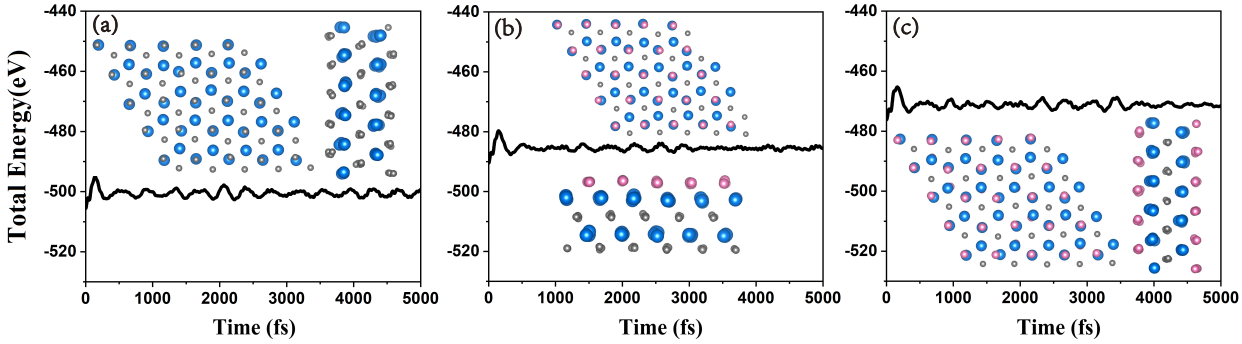

FIG. S2: The AIMD calculations with the total simulation time of 5 ps and an interval of 1 fs of (a) Bi_2Se_3, (b) Bi_2Se_2Te and (c) Bi_2SeTe_2 at T = 300 K. Inserted are the final structures of three monolayer materials from top view and side view.

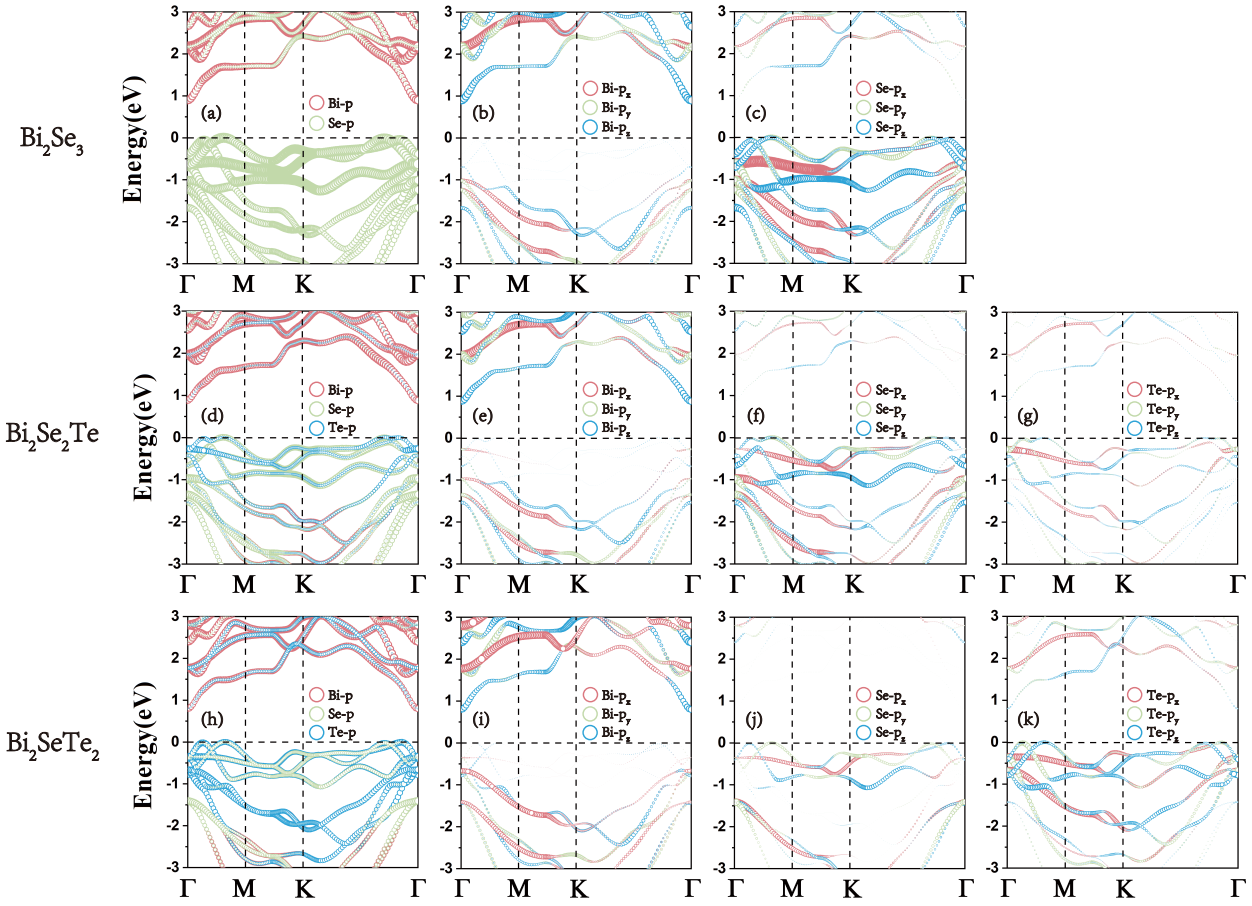

FIG. S3: The site and orbital-projected band structure of monolayer Bi_2Se_3 (a-c), Bi_2Se_2Te (d-g) and Bi_2SeTe_2 (h-k). The red, green and blue circles represent p orbitals of Bi, Se and Te atoms in (a,d,h), while represent p_x, p_y and p_z orbitals in the rest of the diagram.

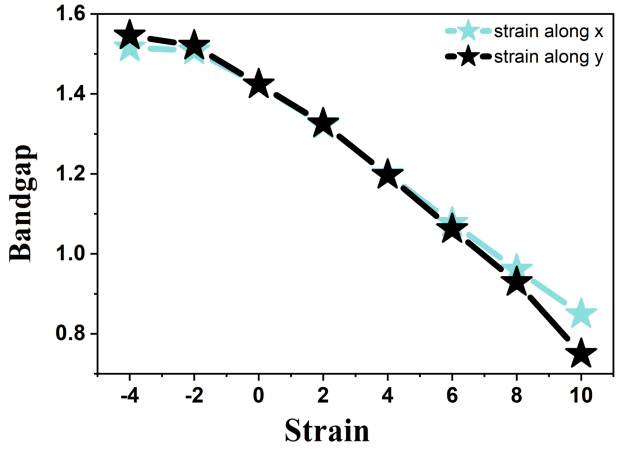

FIG. S4: HSE calculations of the evolution of band gaps for monolayer Bi_2Se_3 as a function of the applied uniaxial strain along the a and b direction.

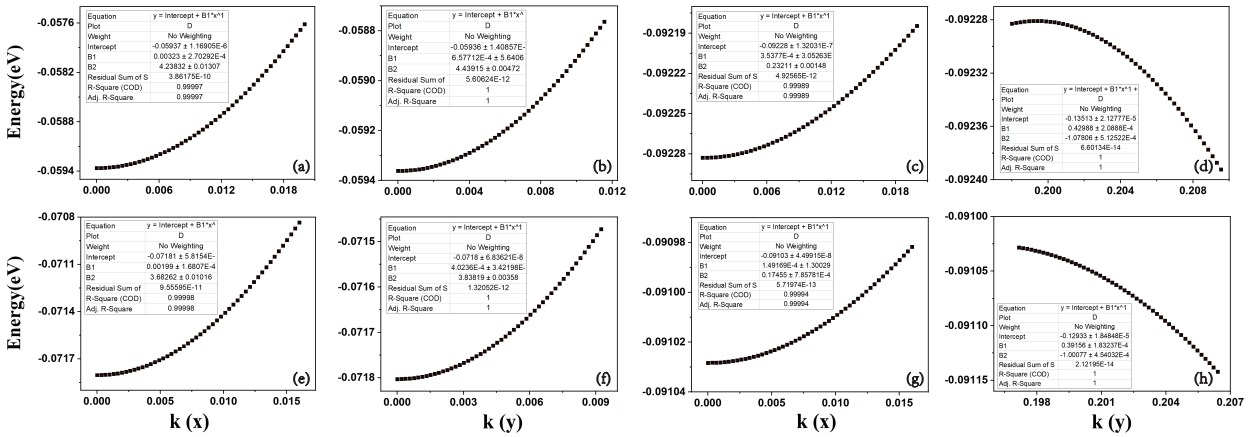

FIG. S5: The m^* fitting diagram of Bi_2Se_3 calculations of PBE in electron (a,b) and hole (c,d), PBE+SOC in electron (e,f) and hole (g,h). The inserted table is the data for the fitting curve.

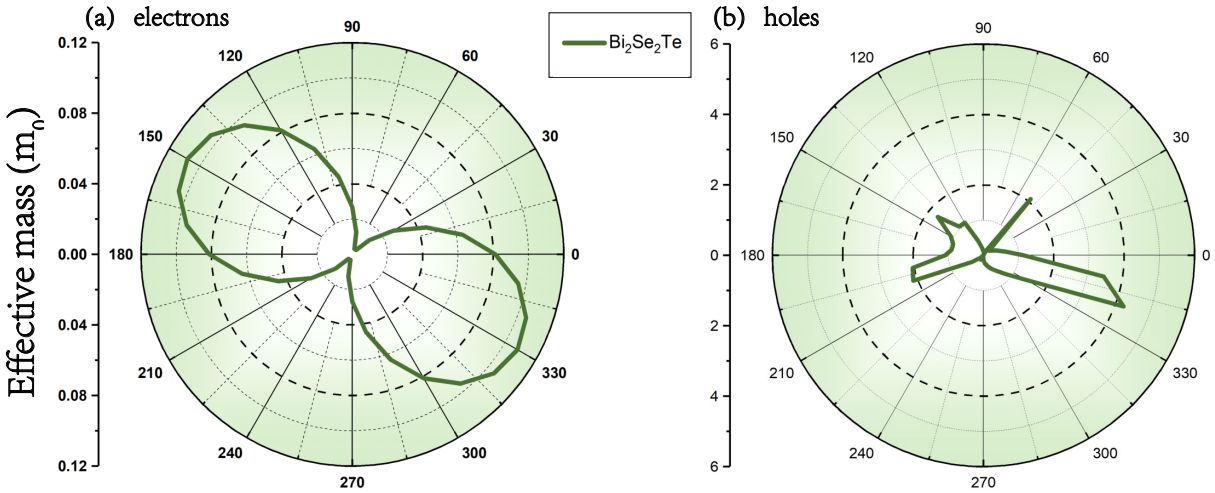

FIG. S6: Angular dependence on the effective masses of (a) electrons and (b) holes for monolayer Bi_2Se_2Te.