Supporting Information for

High Mobility and Ultra-low Lattice Thermal Materials of Monolayer ZnX_2Z_4 (X=In, Al, Ga; Z=S, Se, Te)

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Table S1. Cohesive energy for β_2-ZnX_2Z_4 (X= In, Al, and Ga; Z = S, Se, and Te) was obtained by PBE level.

Structure	E_{coh}(eV)/atom	Structure	E_{coh}(eV)/atom	Structure	E_{coh}(eV)/atom
β_2-$ZnIn_2S_4$	-3.076	β_2-$ZnAl_2S_4$	-3.965	β_2-$ZnGa_2S_4$	-3.457
β_2-$ZnIn_2Se_4$	-2.873	β_2-$ZnAl_2Se_4$	-3.460	β_2-$ZnGa_2Se_4$	-3.022
β_2-$ZnIn_2Te_4$	-2.493	β_2-$ZnAl_2Te_4$	-2.895	β_2-$ZnGa_2Te_4$	-2.577

Table S2. The Elastic constants C_{ij} of the β_2-ZnX_2Te_4 (X= Al, Ga, and In) monolayer.

Monolayer	C_{11} (N/m)	C_{12} (N/m)	C_{22} (N/m)	C_{66} (N/m)
β_2-$ZnAl_2Te_4$	86.19	30.84	89.43	29.58
β_2-$ZnGa_2Te_4$	83.13	32.74	86.33	27.43
β_2-$ZnIn_2Te_4$	63.13	28.11	67.87	20.05

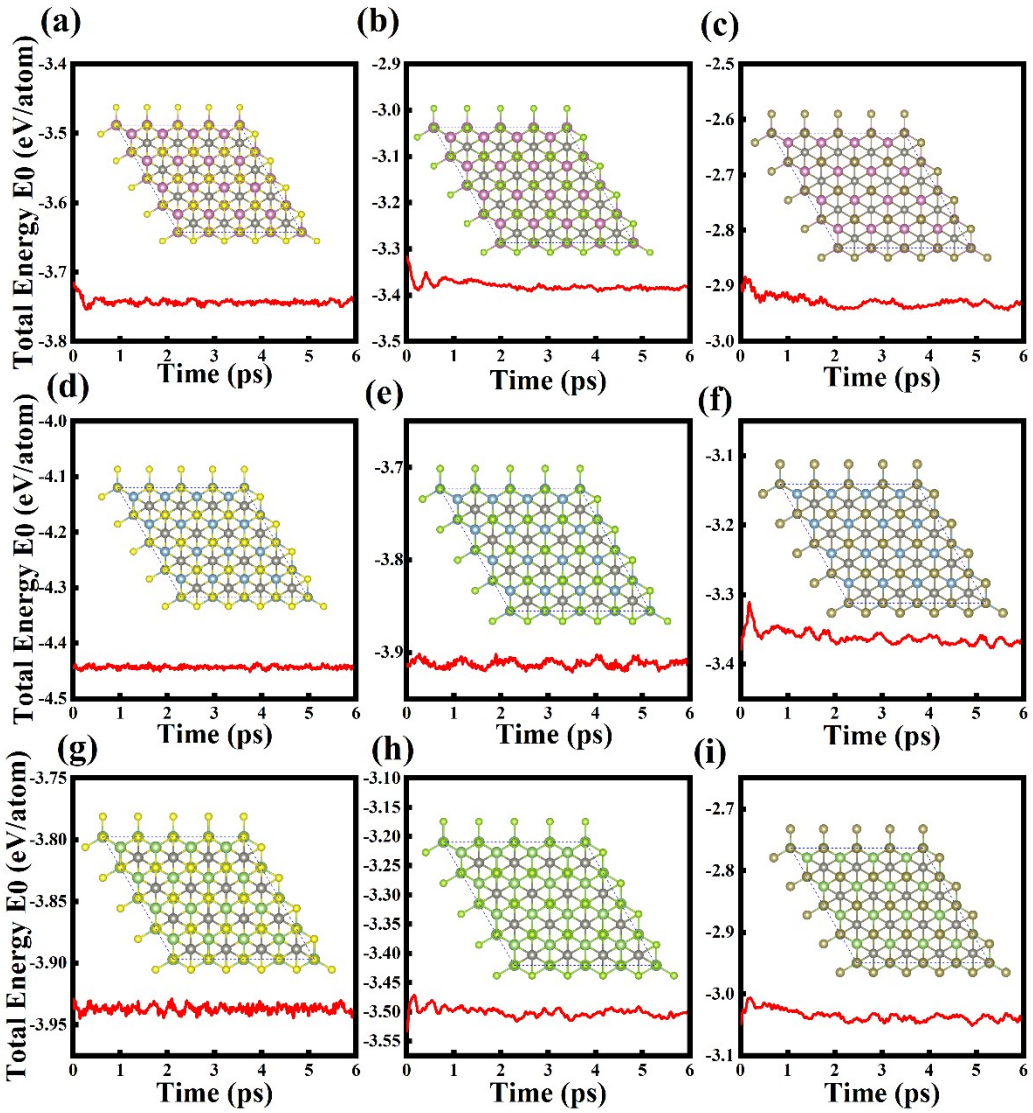

Figure S1. AIMD simulation of 6 ps in (a) β_2-$ZnIn_2S_4$, (b) β_2-$ZnIn_2Se_4$, (c) β_2-$ZnIn_2Te_4$, (d) β_2-$ZnAl_2S_4$, (e) β_2-$ZnAl_2Se_4$, (f) β_2-$ZnAl_2Te_4$, (g) β_2-$ZnGa_2S_4$, (h) β_2-$ZnGa_2Se_4$,and (i) β_2-$ZnGa_2Te_4$ at 300 K.

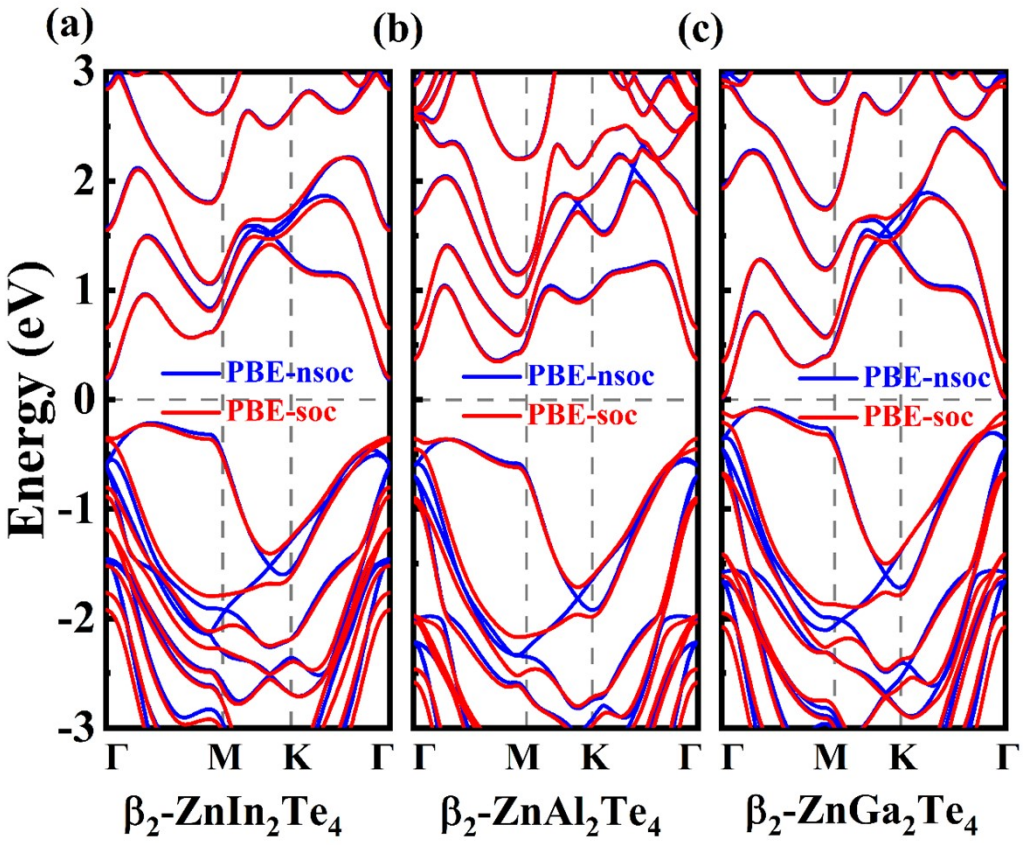

Figure S2. (a-c) The calculated band structure without (blue line) and with (red line) SOC of monolayer β_2-ZnX_2Te_4 (X=In, Al and Ga) by PBE level.

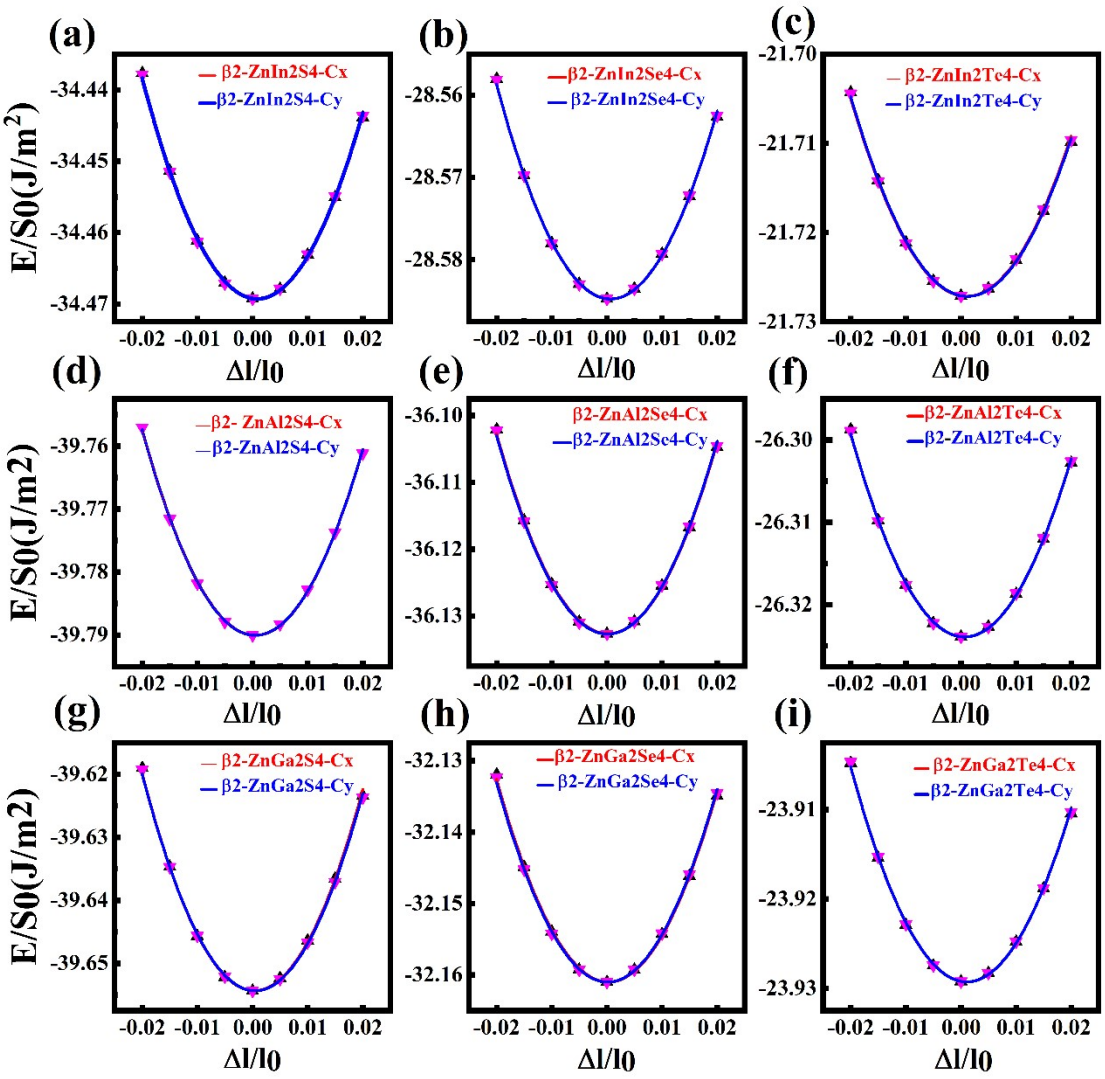

Figure S3. Monolayer (a) β_2-$ZnIn_2S_4$, (b) β_2-$ZnIn_2Se_4$, (c) β_2-$ZnIn_2Te_4$, (d) β_2-$ZnAl_2S_4$, (e) β_2-$ZnAl_2Se_4$, (f) β_2-$ZnAl_2Te_4$, (g) β_2-$ZnGa_2S_4$, (h) β_2-$ZnGa_2Se_4$,and (i) β_2-$ZnGa_2Te_4$ are the x(zigzag) directions of uniaxial strain and the y(armchair) directions of unstrained strain. The in-plane stiffness C_{2D} can be obtained by fitting the parabola.

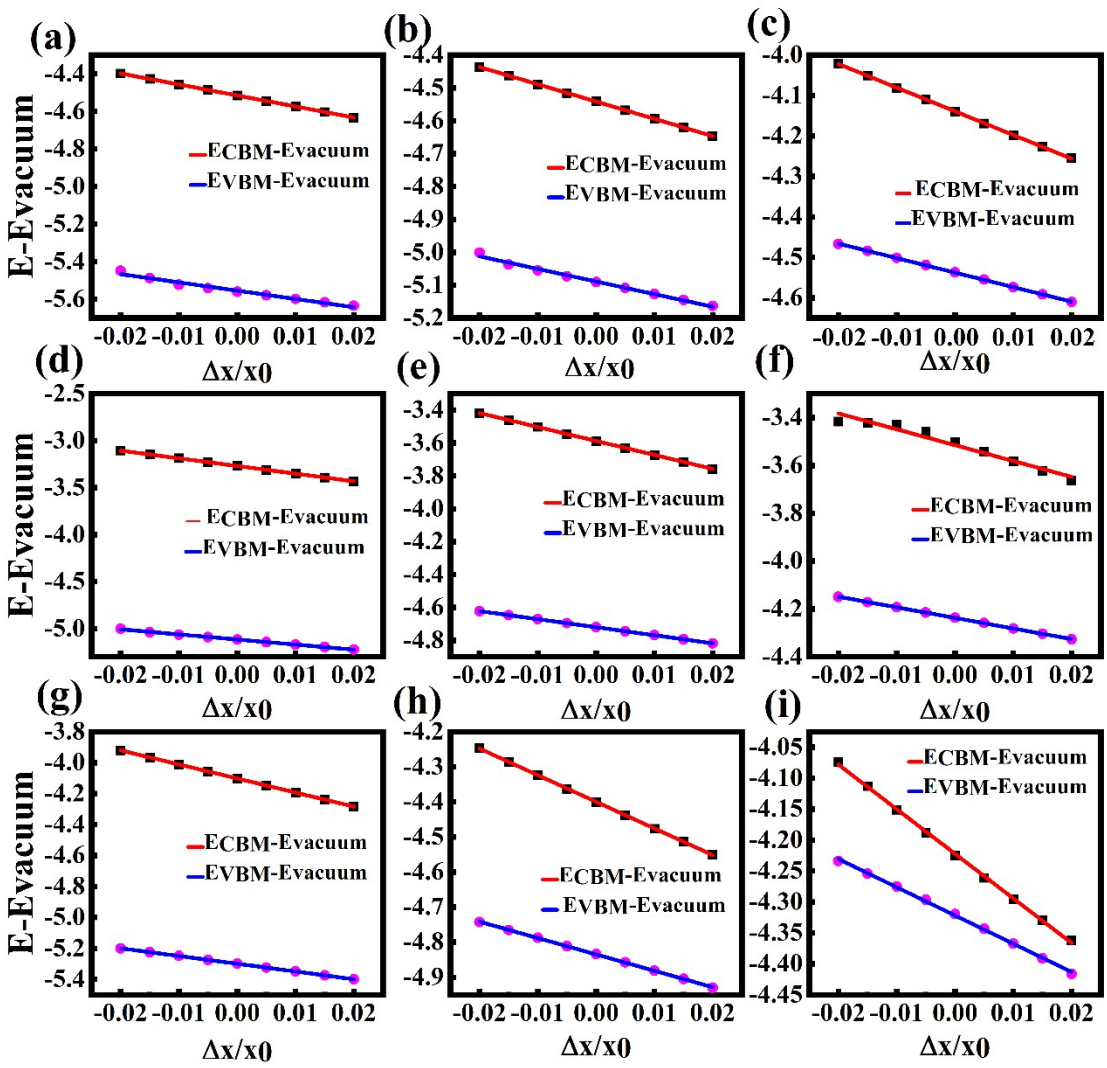

Figure S4. Monolayer (a) β_2-$ZnIn_2S_4$, (b) β_2-$ZnIn_2Se_4$, (c) β_2-$ZnIn_2Te_4$, (d) β_2-$ZnAl_2S_4$, (e) β_2-$ZnAl_2Se_4$, (f) β_2-$ZnAl_2Te_4$, The energy difference and vacuum energy of (g) β_2-$ZnGa_2S_4$, (h) β_2-$ZnGa_2Se_4$, and (i) β_2-$ZnGa_2Te_4$ CBMs and VBMs are functions of lattice expansion along the x(zigzag) direction, respectively. The slope of the blue and red lines corresponds to the DP (Deformation Potential) constant of the hole and electron in a different direction, respectively.

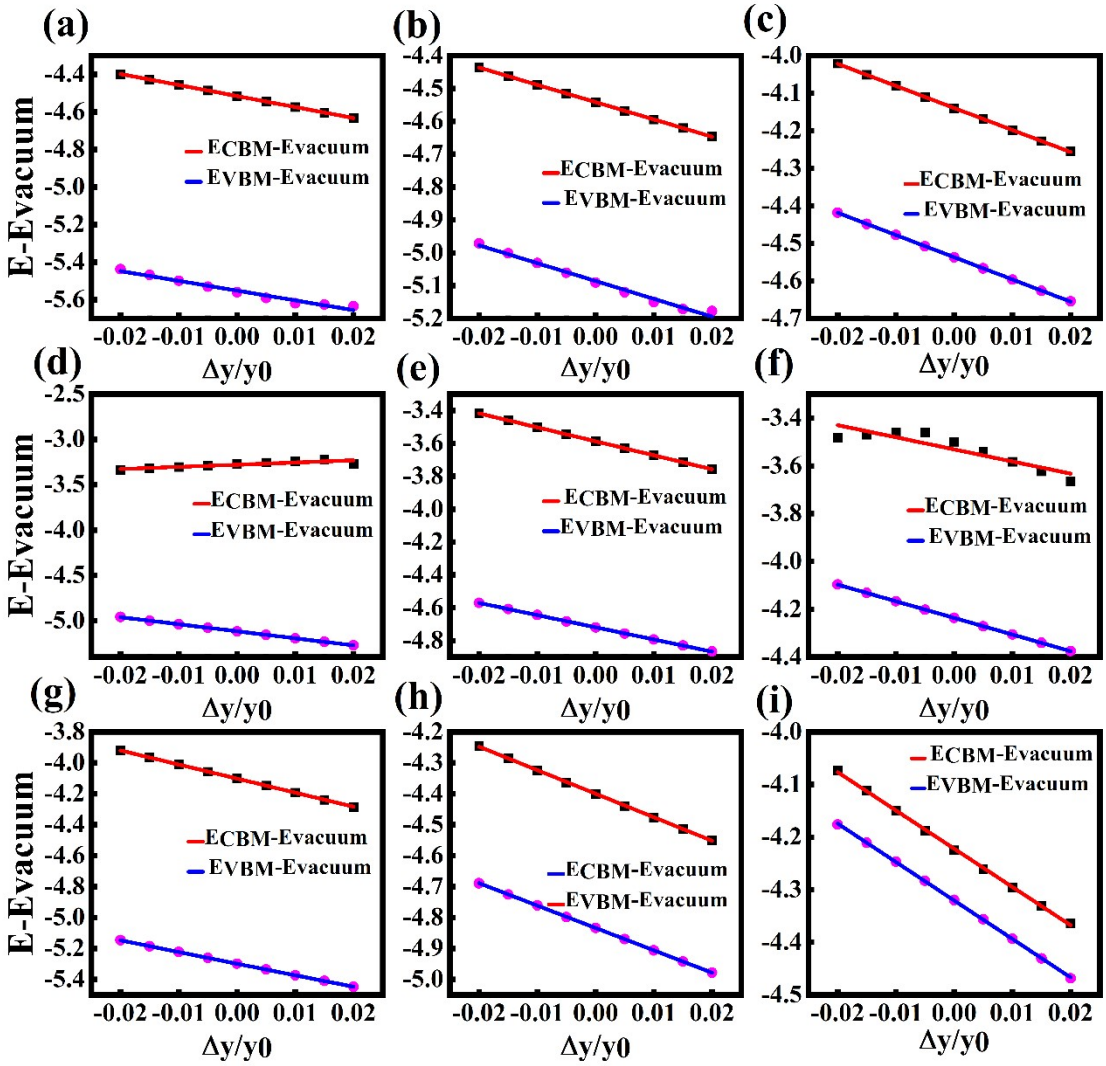

Figure S5. Monolayer (a) β_2-$ZnIn_2S_4$, (b) β_2-$ZnIn_2Se_4$, (c) β_2-$ZnIn_2Te_4$, (d) β_2-$ZnAl_2S_4$, (e) β_2-$ZnAl_2Se_4$, (f) β_2-$ZnAl_2Te_4$, (g) β_2-$ZnGa_2S_4$,(h) β_2-$ZnGa_2Se_4$, and (i) β_2-$ZnGa_2Te_4$ .The energy difference and vacuum energy of CBMs and VBMs are functions of lattice expansion along with the y (armchair) direction, respectively. The slope of the blue and red lines corresponds to the DP (Deformation Potential) constant of the hole and electron in a different direction, respectively.

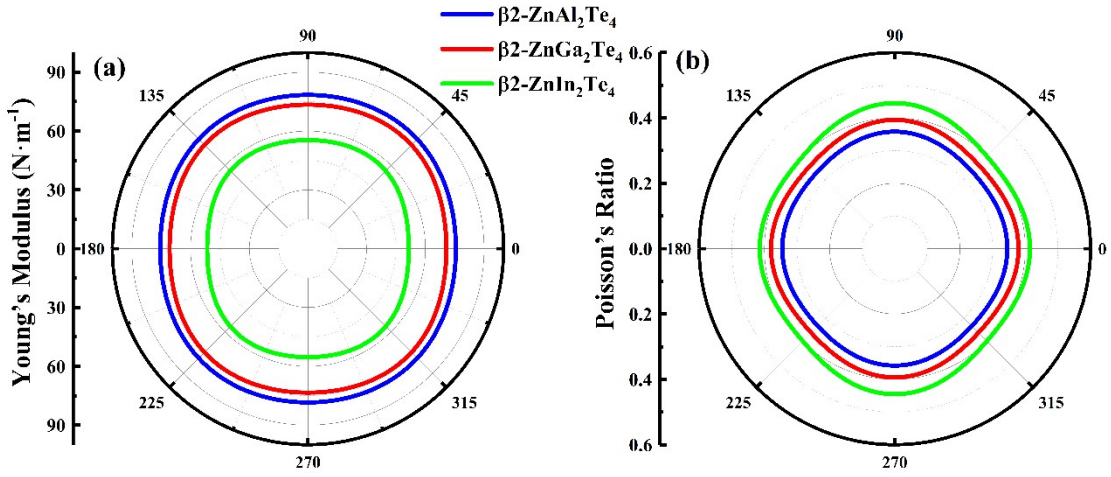

Figure S6. (a) Young's moduli and (b) Poisson's ratio of the β_2-ZnX_2Te_4 (X= Al, Ga, and In) monolayer.

Carrier Mobility calculation.

To investigate the material electron and hole transport properties, here, we use the phonon-limited scattering model of the deformation potential theory proposed by Bardeen and Shockley to predict the carrier mobility of monolayer ZnX_2Z_4 (X = Al, Ga, and In; Z = S, Se, and Te). For the 2D semiconductor system, we used the following equation to calculate the intrinsic carrier mobility of the monolayers:

$$\mu_{2d} = \frac{e\hbar^3 C_{2d}}{K_B T m * m_d (E_1)^2} \#(1)$$

where T, K_B, C_{2d}, E_l, m^* are the temperature, Boltzmann constant, elastic modulus of a uniformly deformed crystal, the variational constant along the transport direction, and the effective masses of electrons and holes, respectively. m^* depends on the energy change of the wave vector k along different transport directions, defined as $m^* = \hbar^2/(\partial^2 E/\partial^2 k)$ $\mathrm{m_d}$ is the average effective mass, which is determined $m_d = \sqrt{m_x m_y}$. The valence band maximum (VBM) of electrons along the transport direction or the conduction band minimum (CBM) of the deformation situation constant E1, determined by $E_x = \Delta E_{lx}/(\Delta l_x/l_{x0})$ and $E_y = \Delta E_{ly}/(\Delta l_y/l_{y0})$. The calculation of the deformation potential C_{2d} and the distortion potential E1 in the paper is based on the equilibrium lattice structure, respectively, along with the uniaxial axis of the in-

plane cell or by applying different values of stretching and compression in the interval from -20% to 20% (taking a series of discrete values at 5% intervals) to achieve the calculation of the cell under different strains.