Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information

The computational process of carrier mobility

The carrier mobility of 2D material is calculated by the deformation potential theory. Owing to the anisotropic in TI materials, it needs to be considered from the x and y directions during the analog computation. Firstly, the material models should change the rhombohedral crystal system into orthorhombic by redefining the lattice because this is convenient for models to apply strains along the x and y directions. The associated models and Brillouin zones selected in calculation are shown in Fig S1.

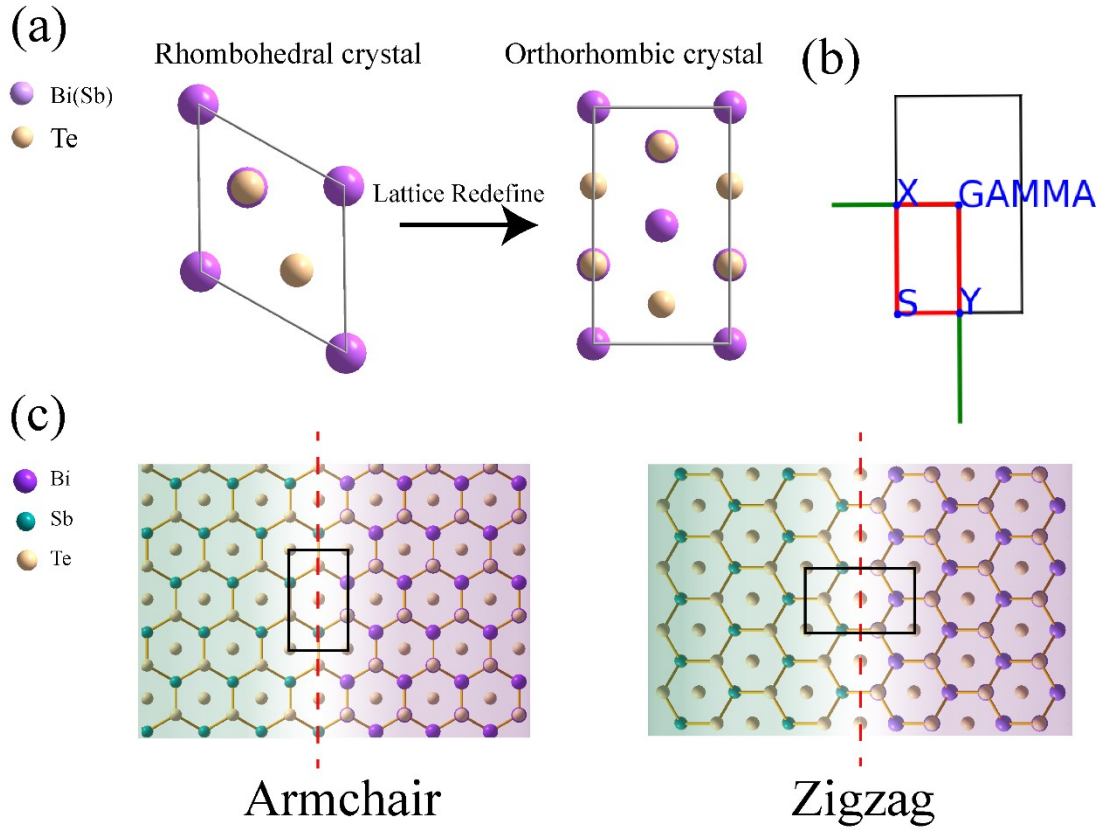


Fig S1. (a) The crystal change of model for computation. (b) Brillouin zone of model for computation. (c) The lateral heterostructure (LHS) models of armchair and zigzag type for computation.

After finishing the building of the material models, the geometry optimization was executed according to the initial parameters. Then a series of strains from -2% to 2% (calculated using a step of 0.5%) along the x and y directions were separately applied in these four models, including Bi_2Te_3, Sb_2Te_3, LHS of zigzag and armchair type, to make it compression and dilatation by changing the parameters in POSCAR. The total energy of these models in different strains could be acquired by computation. The relation between the strain and total energy was fitted by the quadratic function. The corresponding computation and fitting data of these four models in different strains along the x and y directions were shown in the Fig S2.

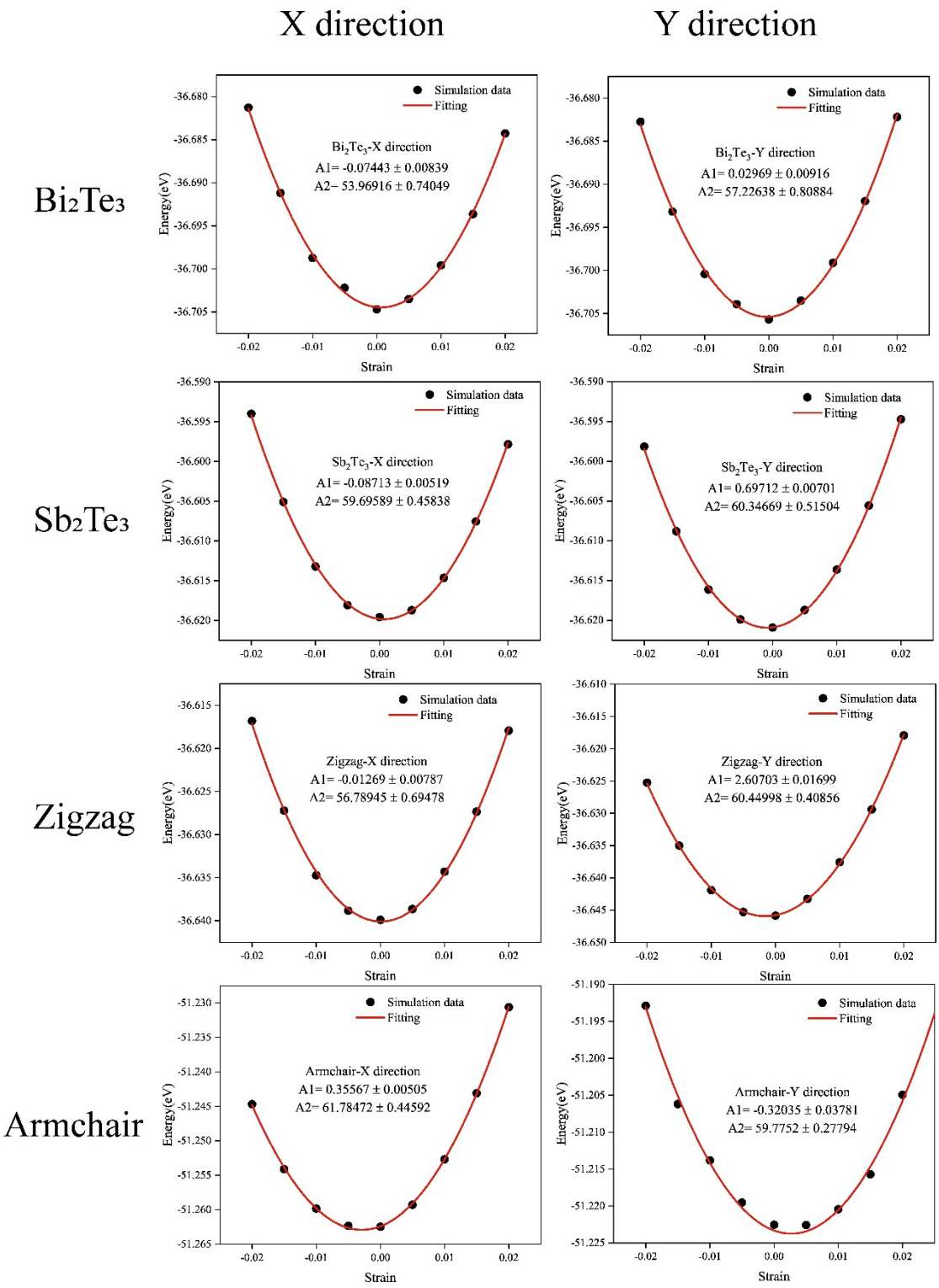


Fig S2. The elastic modulus C of these four models by computation and fitting.

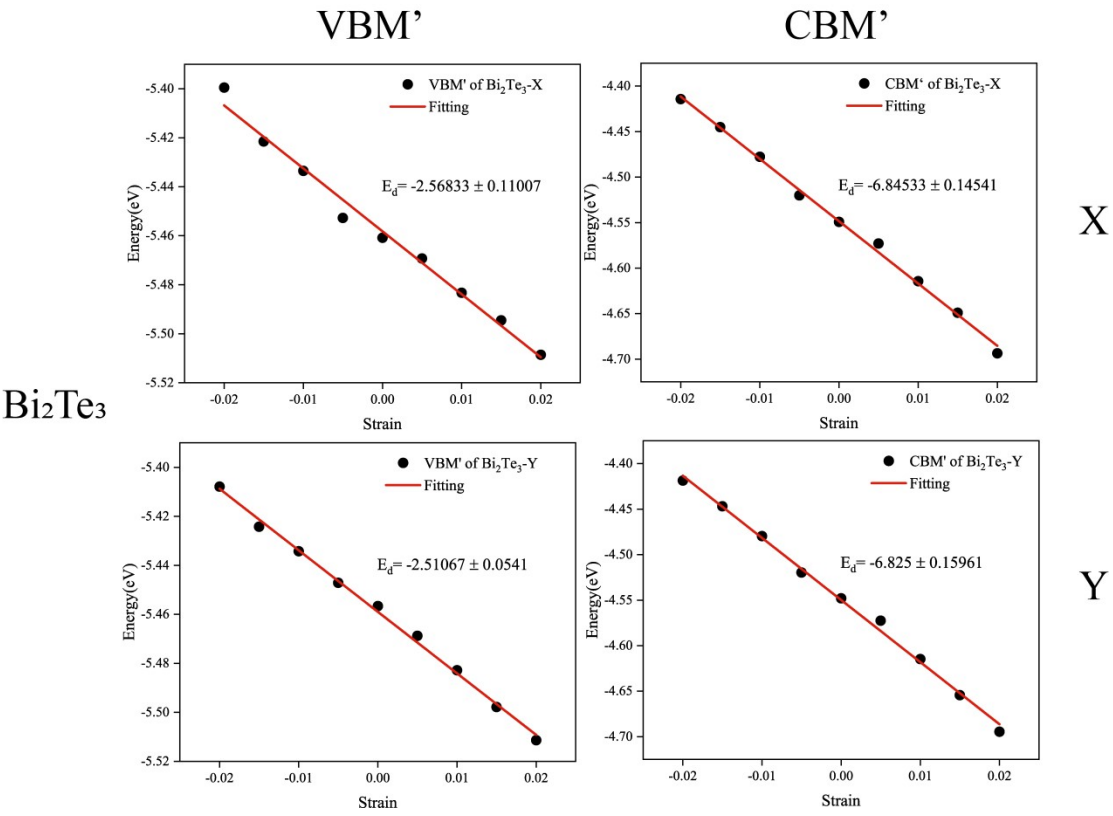
According to the fitting results, the quadratic term ratio A_2 and monomial term ratio A_1 can be acquired. Then the formula $C = \left[\frac{\partial^2 E}{\partial \varepsilon^2}\right]/S_0$ is integrated to $C = 16 \times 2 \cdot A_2/S_0$, where S_0 is surface area of the equilibrium system acquired by the cell

volume. Finally, the elastic modulus of 2D system C can be calculated by the given A_2 and S_0. The associated parameters are listed in the Table S1.

Table S1 The quadratic term ratio A_2, surface area S_0, the elastic modulus C of these four models acquired by the analog computation along the x and y directions.

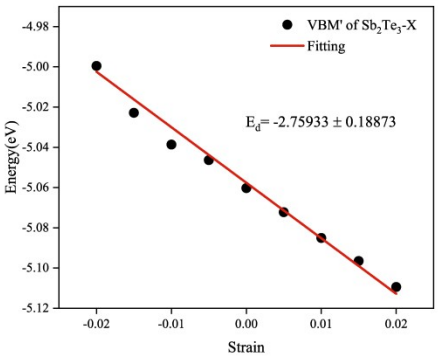
	X			Y		
	A_2	S_0	C	A_2	S_0	C
Bi_2Te_3	53.96916	34.291	50.363	57.22638	34.291	53.403
Sb_2Te_3	59.69589	34.291	55.708	60.34669	34.291	56.315
Zigzag	56.78945	34.291	52.995	60.44998	34.291	56.411
Armchair	61.78472	34.291	57.657	59.7752	34.291	55.782

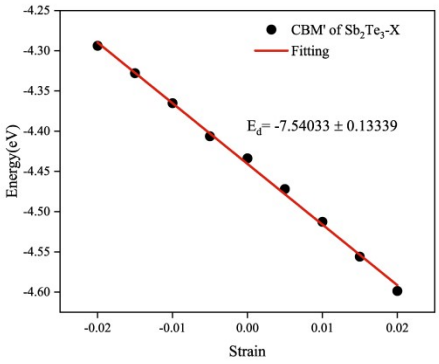
For the deformation potential constant E_d calculation, the initial models after the geometry optimization and other models after applying different strains were calculated by static self-consistent and non self-consistent calculation in turn. The valence band maximum (VBM), conduction band minimum (CBM), fermi level and vacuum level could be obtained from the band structures after calculation. Then the position changes of band edges in different strains could be figured out by using the vacuum level for reference. The energies of VBM and CBM after changing could also be calculated and the changes in different strains could be linear fitted as shown in Fig S3. According to the fitting results, the deformation potential constant E_d was the slope of linear fitting.



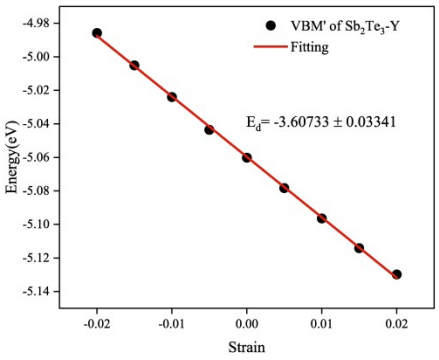
VBM’ CBM’

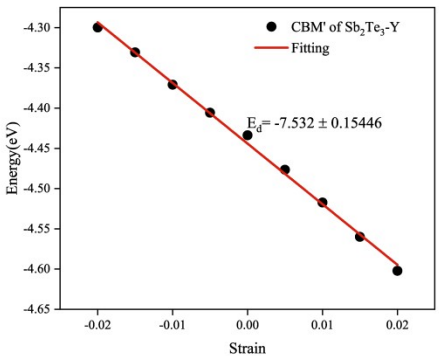
Sb2Te3





X

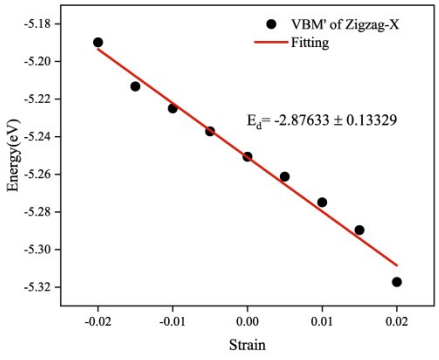


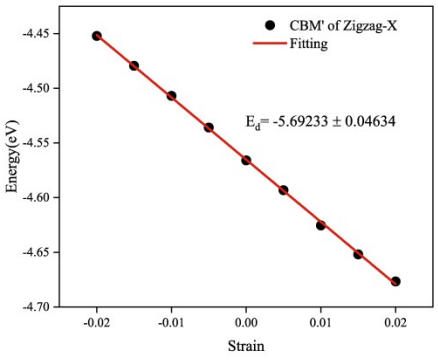


Y

VBM’ CBM’

Zigzag





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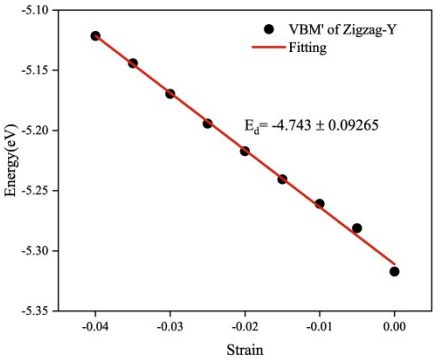

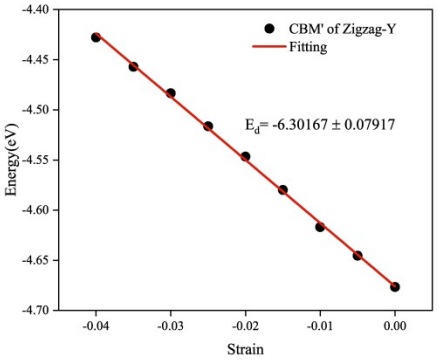

Y

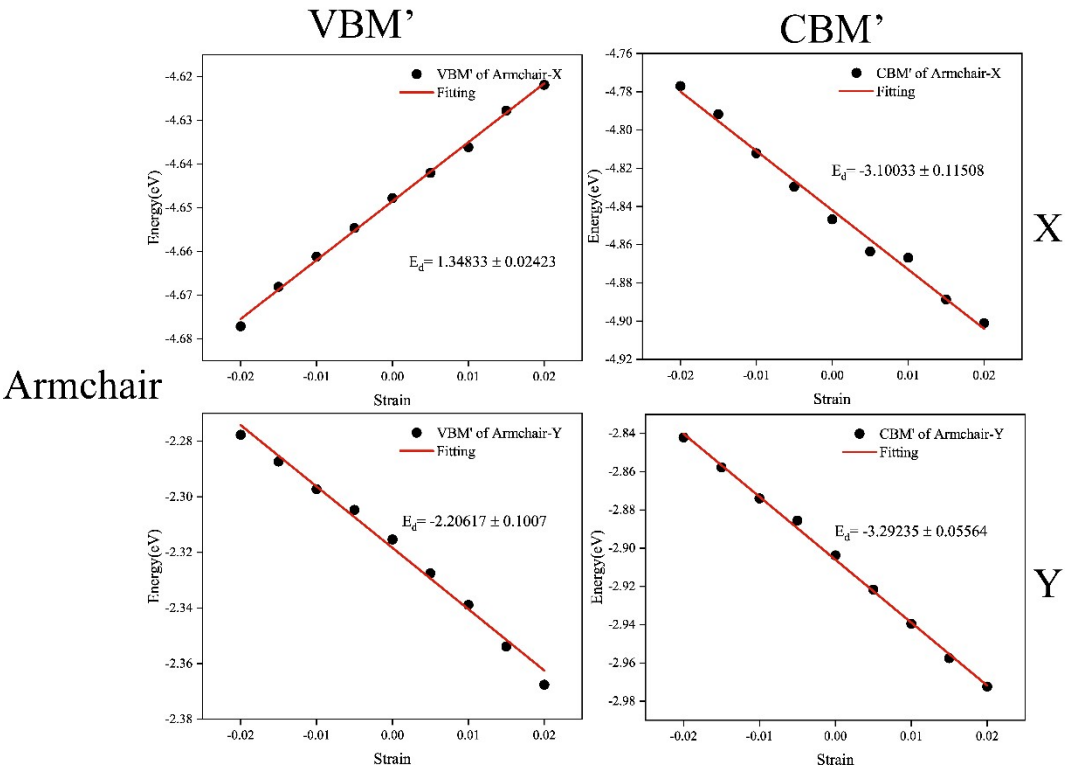

Fig S3. The deformation potential constant E_d of these four models obtained by fitting the relation between the energy of VBM', CBM' after applying the strains and different strains

The carrier effective mass m* is the second derivative of the energy eigenvalue with respect to the high symmetry point K and can be extracted from the band structure calculation along the x and y directions of the VBM and CBM by the vaspkit. The corresponding parameters are listed in the Table S2.

Table S2. The carrier effective mass m* of these four models along the x and y directions.

	m*(m_0)		
		x	y
Bi_2Te_3	h	1.717	0.438
	e	0.094	0.098
Sb_2Te_3	h	0.1	0.099
	e	0.104	0.102
Zigzag	h	0.086	0.091
	e	0.095	0.108
Armchair	h	0.189	0.213
	e	0.154	0.197

Finally, the carrier mobility of 2D material can be figured out by acquired constants C, E_d, m* according the formula $\mu = \frac{2e\hbar^3 C}{3k_B T|m^*|^2 E_d^2}$., where e is the electron charge counted as $1.6 \times 10^{-19} C$, k_B, T, and $\hbar$ are the Boltzman constant, temperature and

reduced Plank constant taken as $1.38 \times 10^{-23} m^2 \cdot kg \cdot s^{-2} \cdot K^{-1}$,$298K$ and $1.055 \times 10^{-34} J \cdot s$, respectively The results are shown in Table S3.

Table S3. The carrier mobility of these four models by calculation.

	$\mu(cm^2 \cdot V^{-1} \cdot s^{-1})$		
		x	y
Bi_2Te_3	h	81.870	648.995
	e	1788.242	1754.792
Sb_2Te_3	h	10757.999	6492.004
	e	1331.759	1402.557
Zigzag	h	12734.373	4451.354
	e	2664.252	1790.098
Armchair	h	13057.679	3713.993
	e	3718.815	1949.662