Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information

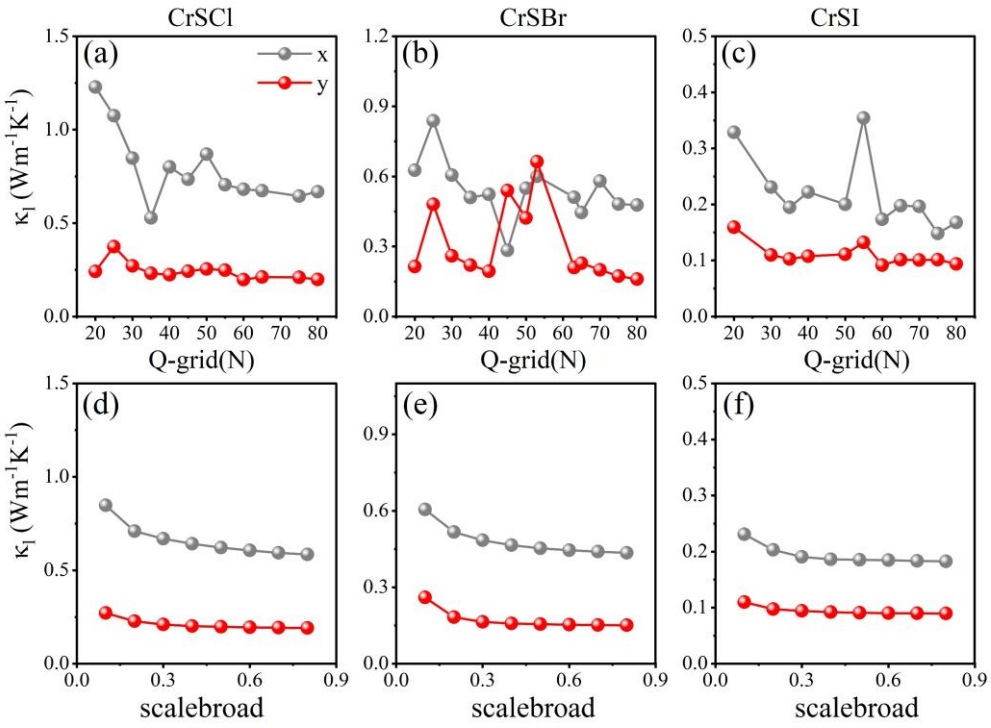

Fig. S1 The first is the experimental results of convergence of thermal conductivity with respect to the nearest Q point. The second section is the experimental results of convergence of thermal conductivity of CrSX monolayers with respect to daub (scale width) parameters.

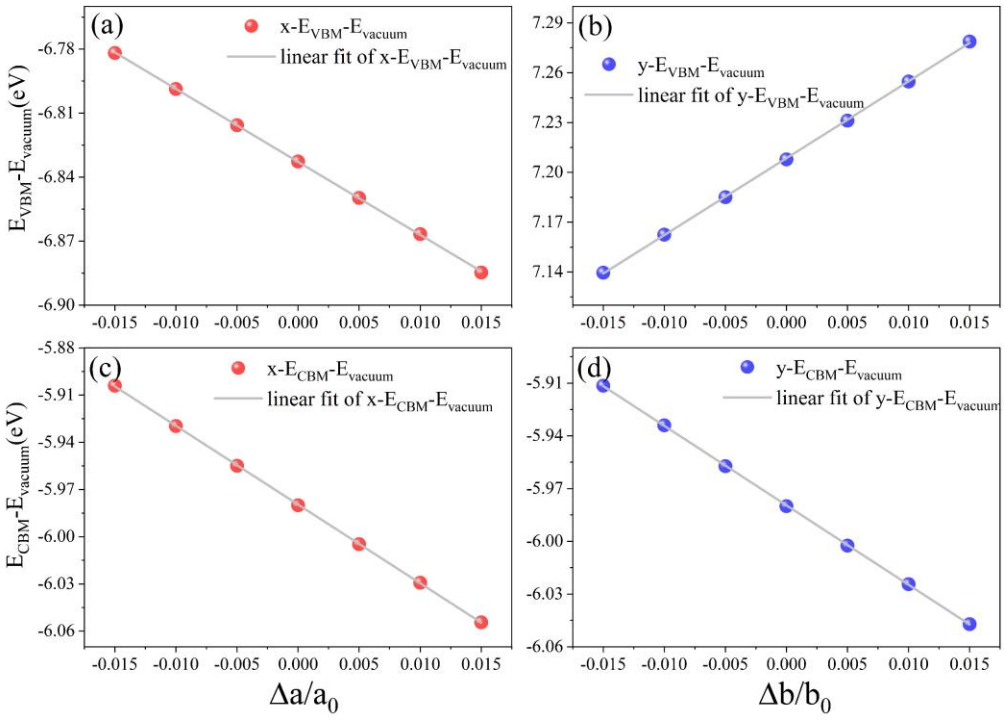

Fig. S2 Band energy with respect to the vacuum energy as a function of lattice dilation for the (a, b) CBM and (c, d) VBM of CrSCl monolayer. Gray solid lines are the fitting curves.

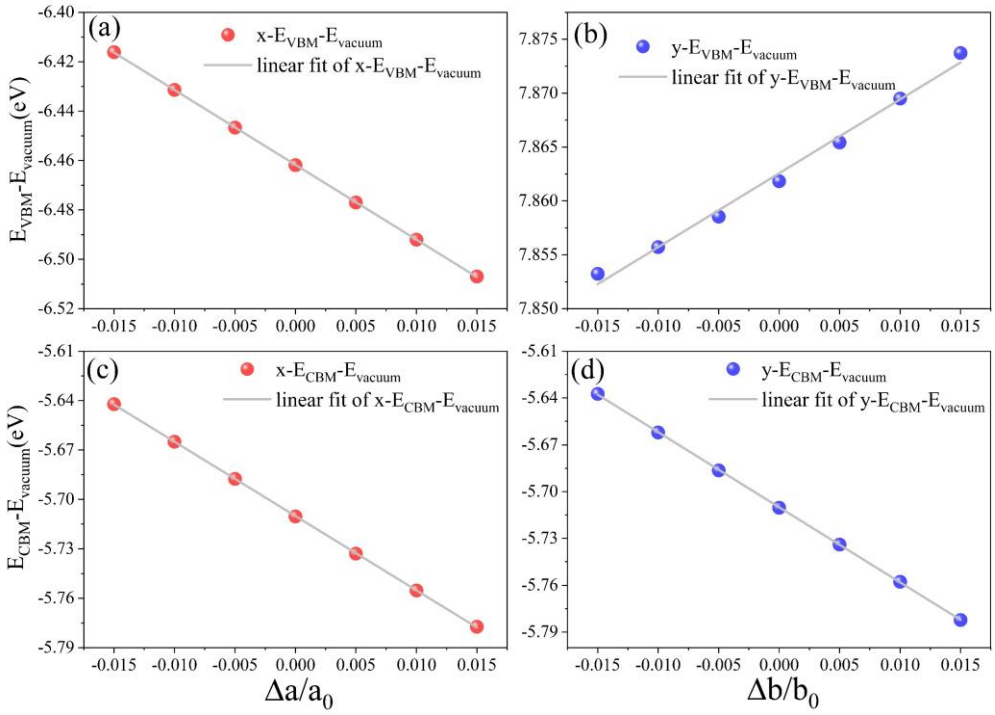

Fig. S3 Band energy with respect to the vacuum energy as a function of lattice dilation for the (a, b) CBM and (c, d) VBM of CrSBr monolayer. Gray solid lines are the fitting curves.

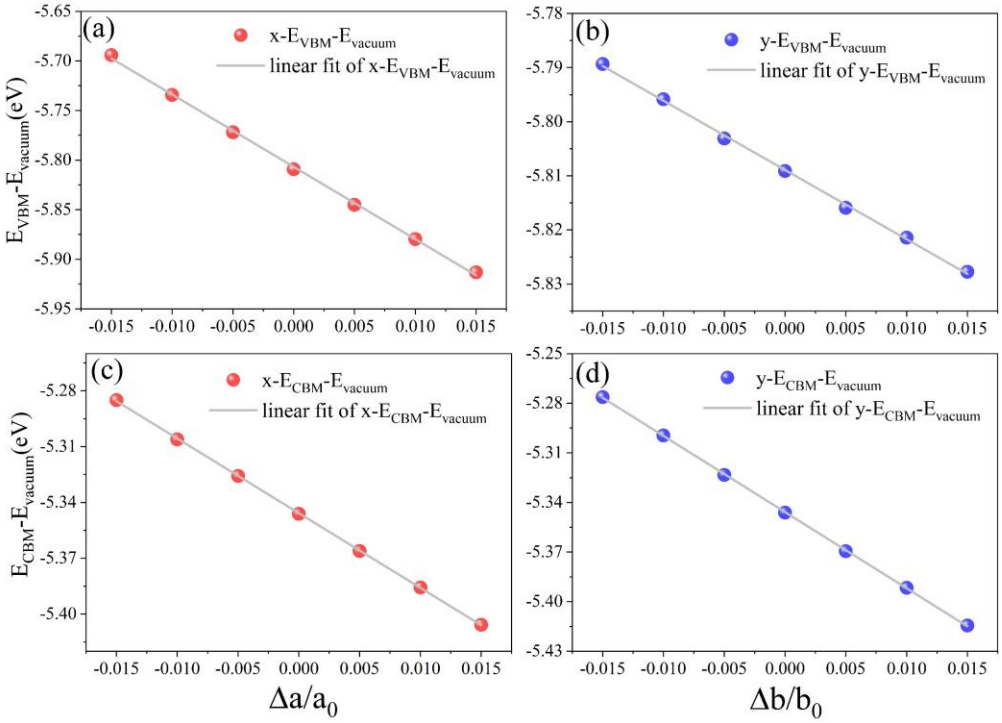

Fig. S4 Band energy with respect to the vacuum energy as a function of lattice dilation for the (a, b) CBM and (c, d) VBM of CrSI monolayer. Gray solid lines are the fitting curves.

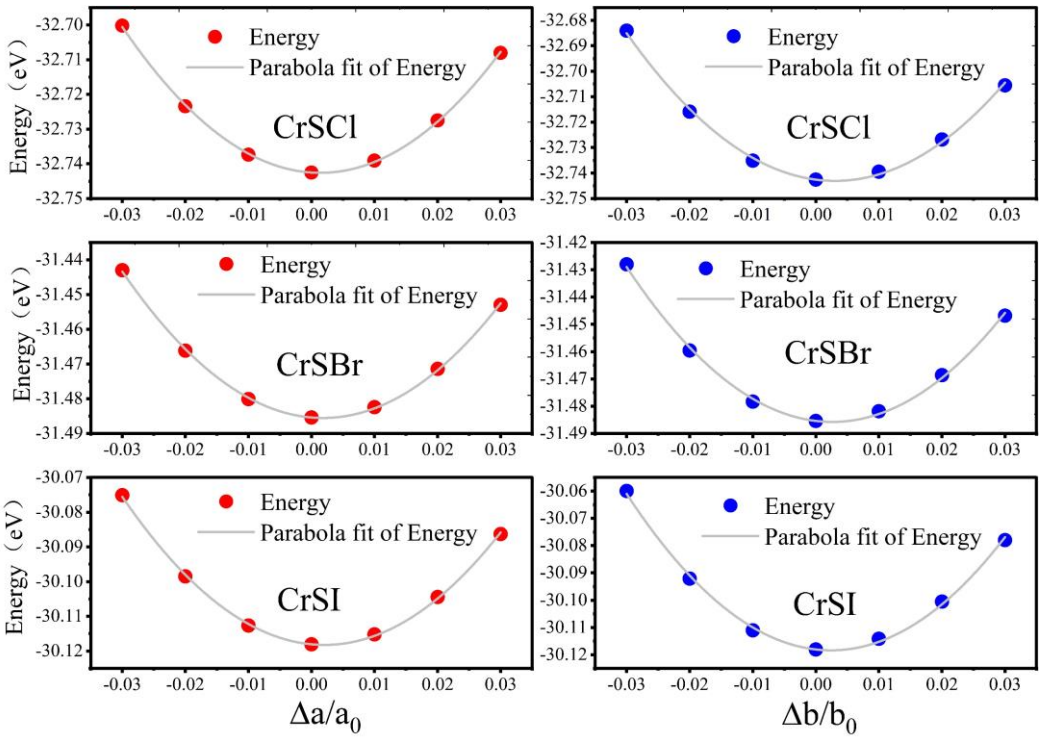

Fig. S5 Total energy-strain curve of CrSX monolayers along the (a, c and e) a and (b, d and f) b directions, respectively.

Table S1 Optimized lattice constant a and b (Å), electronic band gap E_{gap} (eV) of CrSX monolayers.

Name	a	b	E_{gap}
CrSCl	3.48	4.83	1.80
CrSBr	3.58	4.82	1.69
CrSI	3.75	4.80	1.26

Table S2. The calculated elastic constants (C_{ij}) (N/m).

	C_{11}	C_{22}	C_{12}	C_{33}
CrSCl	82.4951791	101.9338301	9.09047097	1.58109603
CrSBr	78.46179433	100.1102892	9.17140177	1.63488964
CrSI	74.95065929	98.1040442	9.1621099	1.39012426

Based on the DPA theory[1], the μ_{2D} and τ in 2D systems can be calculated using the following formula[2]:

$$\mu_{2D} = \frac{e\hbar^3 C^{2D}}{k_B T m_e^* (E_1)^2}, \quad (1)$$

$$\tau = \frac{2\hbar^3 C^{2D}}{3k_B T m_e^* (E_1)^2}, \quad (2)$$

where e, $\hbar$, κ_B, T, C^{2D}, E_1 and m_e^* are the electron charge, the reduced Planck

constant, the Boltzmann constant, the temperature, the 2D elastic modulus, the deformation potential constants and the effective mass along the transport direction.

Table S3

The calculated effective mass (m^*/m_0), deformation-potential constant (E_1, eV), 2D elastic modulus (C^{2D}, $\mathrm{Jm^{-2}}$), relaxation time (τ, fs) and carrier mobility (μ_{2D}, $\mathrm{cm^2V^{-1}s^{-1}}$) for CrSX monolayers at 300 K using old and new formulas (where "old" and "new" denote the use DPA theory and modified DPA method).

Name	type	Direction	m^*/m_0	C^{2D}	E_1	old-τ	new-τ	old-μ	new-μ
CrSCl	h	Γ-X	6.554	81.1	3.42	8.546	97.792	27.844	26.243
		Γ-Y	0.080	101.0	4.63	475.734	88.940	1550.051	1955.372
	e	Γ-X	5.982	81.1	5.00	4.381	32.062	8.067	9.427
		Γ-Y	0.343	101.0	4.52	116.425	35.621	214.393	182.657
CrSBr	h	Γ-X	7.118	77.1	3.03	9.530	123.511	28.155	30.519
		Γ-Y	0.091	98.8	3.51	710.647	122.068	2099.428	2359.297
	e	X-Γ	7.962	77.1	4.51	3.846	24.610	5.200	5.436
		X-S	0.478	98.8	4.81	72.166	25.355	97.576	93.295
CrSI	h	Γ-X	0.280	73.7	7.29	40.008	30.983	87.587	194.620
		Γ-Y	4.888	96.9	1.28	97.739	62.733	213.973	22.573
	e	X-Γ	3.987	73.7	4.01	9.286	50.456	22.396	22.258
		X-S	0.300	96.9	4.61	122.771	50.399	296.106	295.477

References

1. Bardeen, J. & Shockley, W. Deformation Potentials and Mobilities in Non-Polar Crystals. *Phys. Rev.* **80**, 72–80 (1950).
2. Zhang, L.-C. *et al.* Tinselenidene: a Two-dimensional Auxetic Material with Ultralow Lattice Thermal Conductivity and Ultrahigh Hole Mobility. *Sci. Rep.* **6**, 19830 (2016).