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

Thermoelectric Properties of Two-Dimensional Selenene and Tellurene from Group-VI Elements

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1. PBE-SOC and HSE band structures:

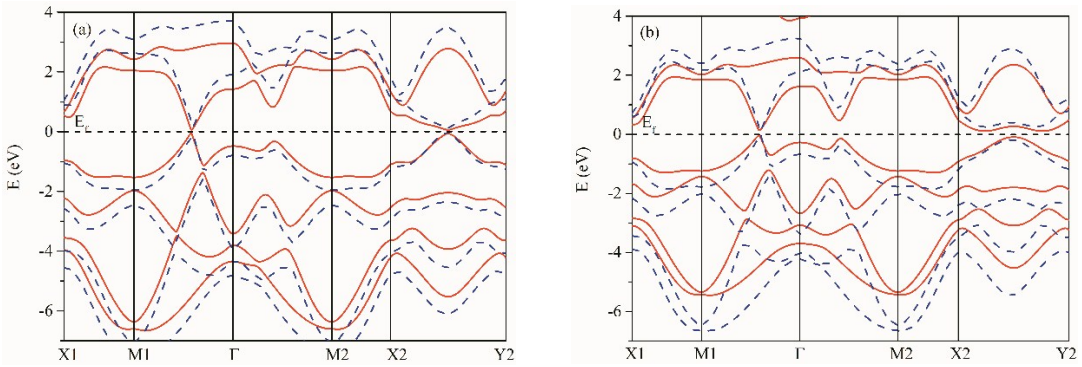


Figure S1. Electronic band structure calculated with PBE-SOC (red line) and HSE (dash blue line) for (a) selenene and (b) tellurene.

2. Effective mass fitting

The effective mass m^* is given as

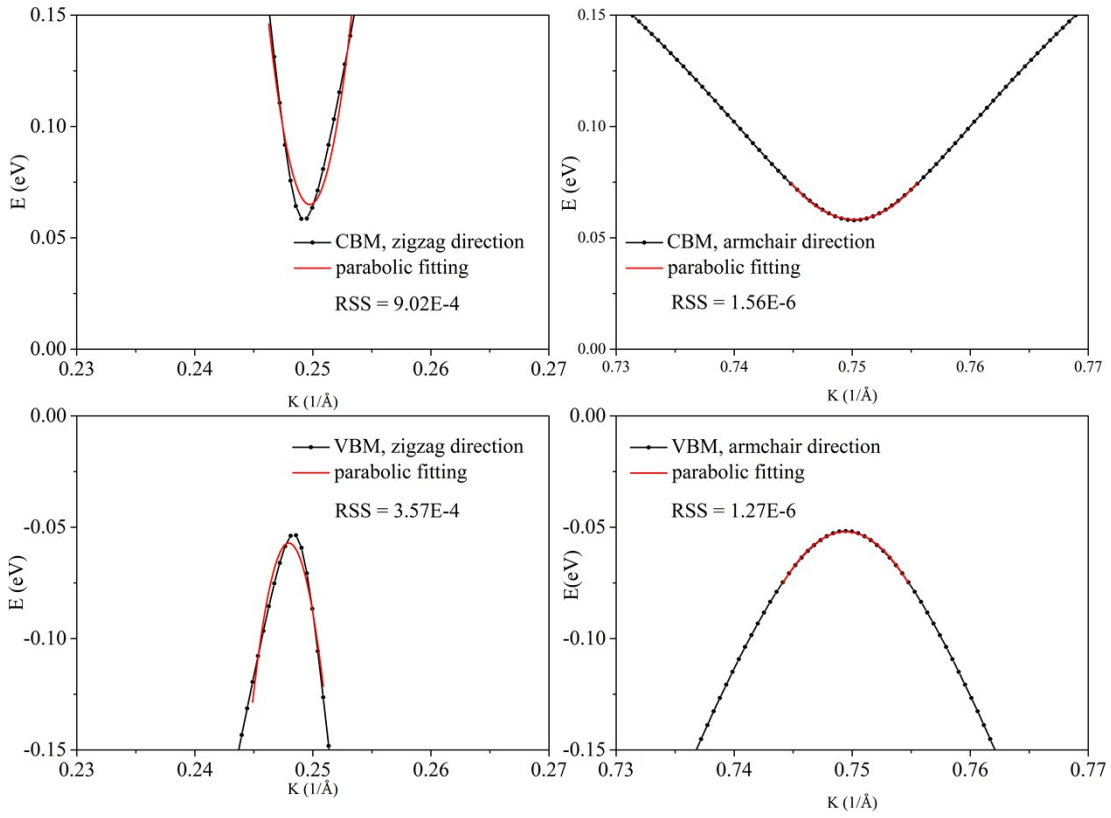
$$m^* = \left(\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right)^{-1}$$

Where $\hbar$ is reduce Planck constant, E is band energy, and k is reciprocal k-space.

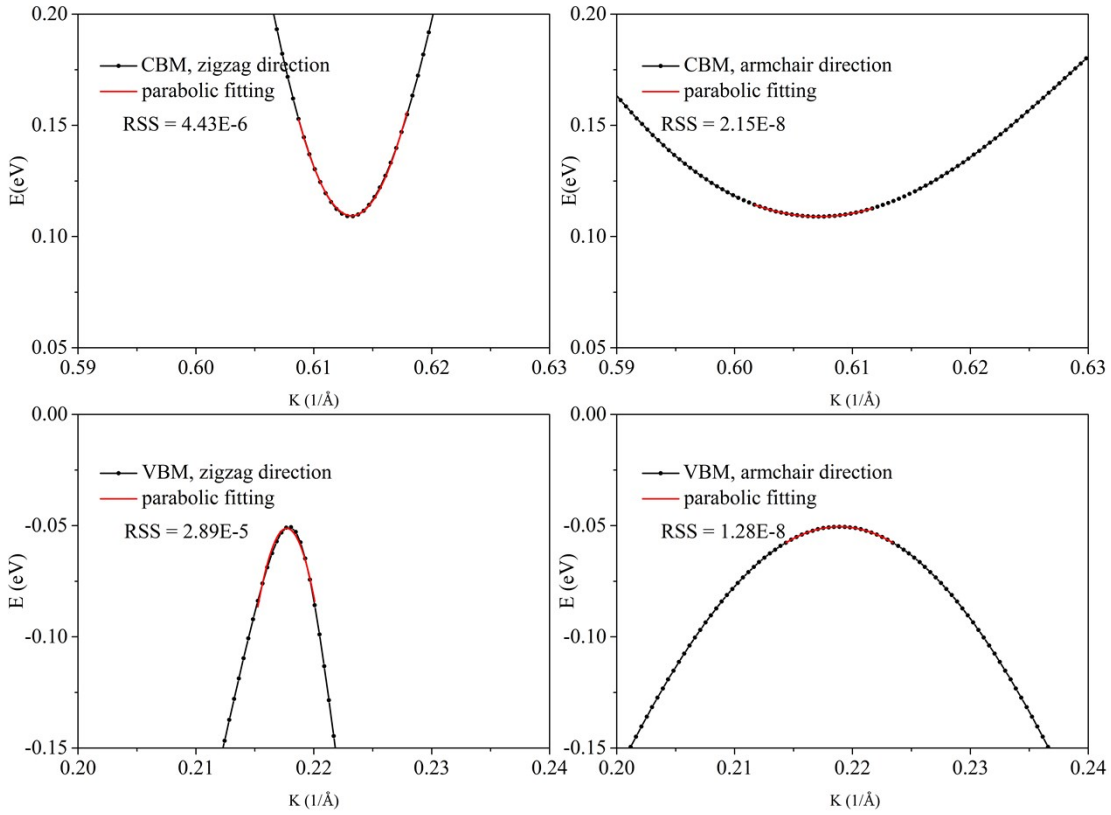
The parabolic fitting range is shown in **Figure S1** and the fitting parameter is given in **Table S1**.

TABLE S1. Parabolic fitting B2 parameters (equation: y = intercept + B1*X + B2*X^2, energy: eV, length: Å) for the effective mass calculated by PBE-SOC and HSE (in parenthesis) method for selenene and tellurene

2D material	Band	zigzag	Armchair
Selenene	conduction	6742	575
		(6777)	(684)
	Valance	-7569	-816
		(-9227)	(-798)
Tellurene	conduction	2124	178
		(2707)	(188)
	Valance	-5835	-349
		(-7554)	(-368)



(a)



(b)

Figure S2. Parabolic fitting for (a) selenene and (b) tellurene calculated with PBE-SOC. 16~20 points around the minimum (maximum) point is used to fit. RSS: Residual Sum of Squares