Supplementary Materials for

Topological and superconducting properties in two-dimensional *MX*C_3 [*M*:*X* = In:As, Se:As, In:Te and As:Te] by First-principle study

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I. Computational details on electronic susceptibility, phonon linewidth and superconductivity

The Eliashberg spectral function [1,2]:

$$\alpha^2F(\omega) = \frac{1}{N(E_F)N_kN_q}\sum_{\mathbf{k},q,\nu,i,j} |g_{\mathbf{k}i,\mathbf{k+q}j}^{\mathbf{q}\nu}|^2\delta(\omega - \omega_{\mathbf{q}\nu}) \times \delta(\epsilon_{\mathbf{k}i} - E_F)\delta(\epsilon_{\mathbf{k+q}i} - E_F), \tag{1}$$

where N(E_F) is the electronic DOS at the Fermi level, N_k and N_q represent the total number of **k** points and **q** points respectively. $\omega_{\mathbf{q}\nu}$ is the phonon frequency of the νth phonon mode at vector **q**, $\epsilon_{\mathbf{k}i}$ and $\epsilon_{\mathbf{k+q}i}$ mean the Kohn-Sham energy, $|g_{\mathbf{k}i,\mathbf{k+q}i}^{\mathbf{q}\nu}|^2$ is the electron-phonon coupling matrix element.

The EPC function $\lambda(\omega)$ with the following equation:

$$\lambda(\omega) = 2\int_0^\infty \frac{\alpha^2F(\omega)}{\omega}\,d\omega, \tag{2}$$

The McMillan equation modified by Allen Dynes [3] is

$$T_c = \frac{\omega_{log}}{1.2}\exp\left[\frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right], \tag{3}$$

where μ^* is the Coulomb pseudopotential, μ^* is set to 0.1 [4], ω_{log} is logarithmically averaged frequency and is defined as:

$$\omega_{log} = \exp\left[\frac{2}{\lambda}\int_0^\omega \alpha^2F(\omega)\frac{\log\omega}{\omega}d\omega\right]. \tag{4}$$

For the strong EPC cases, *i.e.*, $\lambda > 1.3$, T_c is estimated [3] by

$$T_c^{AD} = f_1f_2\frac{\omega_{log}}{1.2}exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right]. \tag{5}$$

Here, f_1 and f_2 are the strong-coupling correction factor and the shape correction factor, respectively, with

$$f_1f_2 = \sqrt[3]{1+(\frac{\lambda}{2.46(1+3.8\mu^*)})^{\frac{3}{2}}} \times (1 - \frac{\lambda^2(1-{\omega_2}/{\omega_{log}})}{\lambda^2+3.312(1+6.3\mu^*)^2}) \tag{6}$$

in which ω_2 is defined as

$$\omega_2 = \sqrt{\frac{1}{\lambda}\int_0^{\omega_{max}}[\frac{2a^2F(\omega)}{\omega}]\omega^2d\omega} \tag{7}$$

II. 3D electronic local area map for *MX*C_3.

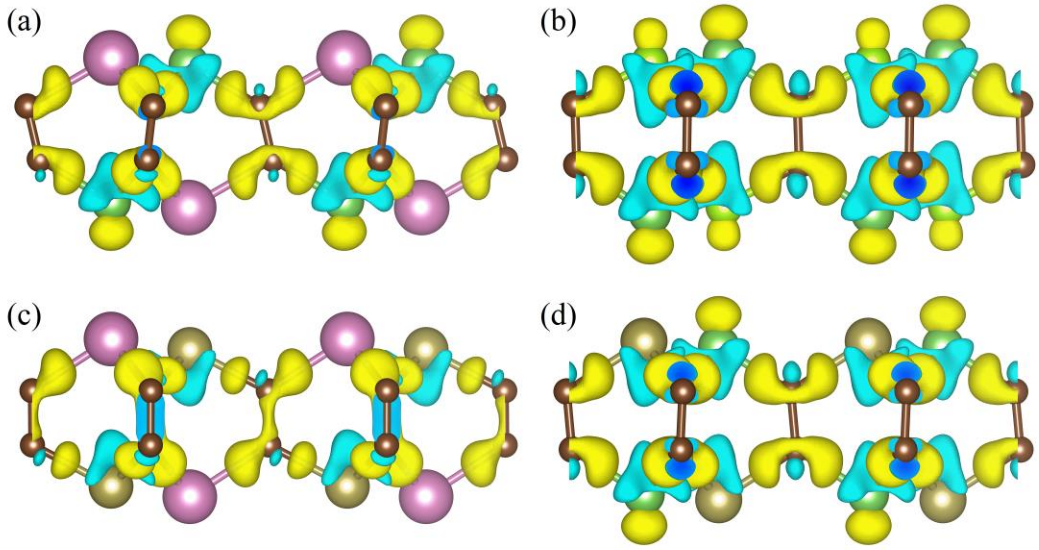

Fig. S1: Charge density difference of (a) $InAsC_3$, (b) $SeAsC_3$, (c) $InTeC_3$ and (d) $AsTeC_3$.

III. The dynamic stability of $InTeC_3$

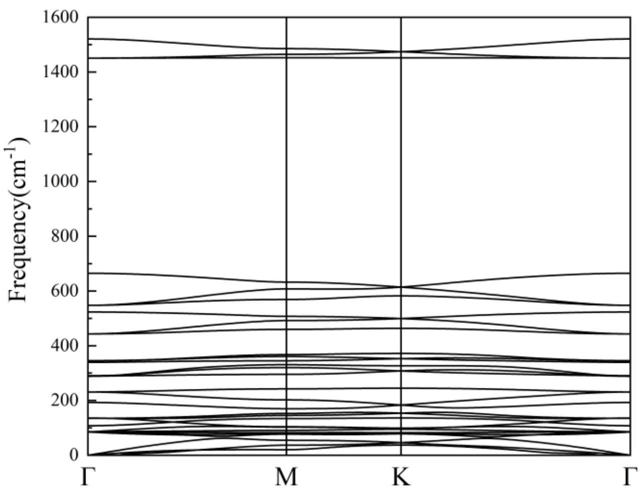

Fig. S2: Phonon spectra of $InTeC_3$.

IV. The band, DOS and PDOS of $InTeC_3$

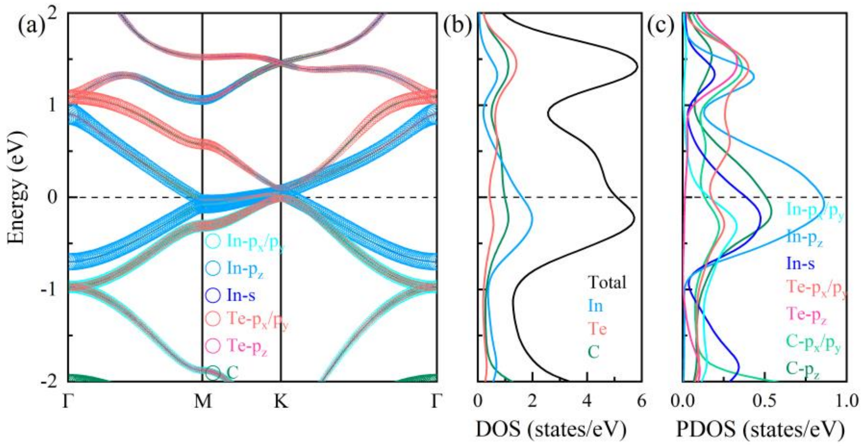

Fig. S3: Band (a), DOS (b) and PDOS (c) for $InTeC_3$.

V. The band without and with SOC of $InTeC_3$, and corresponding topological edge states

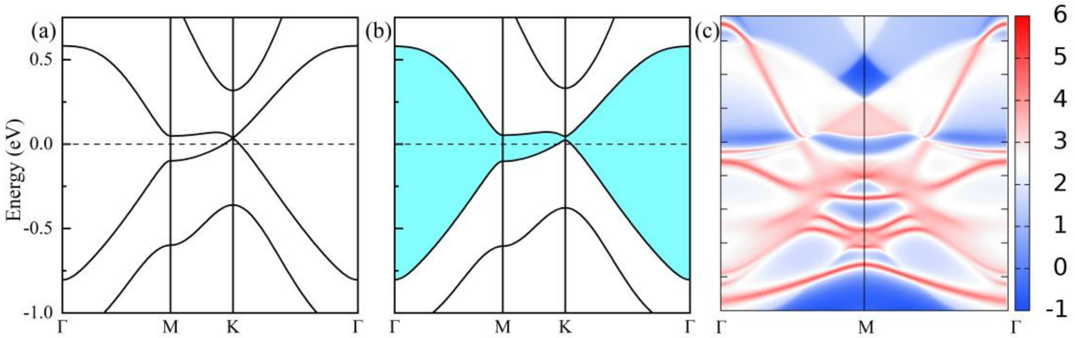

Fig. S4: Comparison of band maps without SOC (a), with SOC (b) and corresponding topological edge states (c). The topological edge states in the (01) edge.

VI. The band, DOS and PDOS of $AsTeC_3$

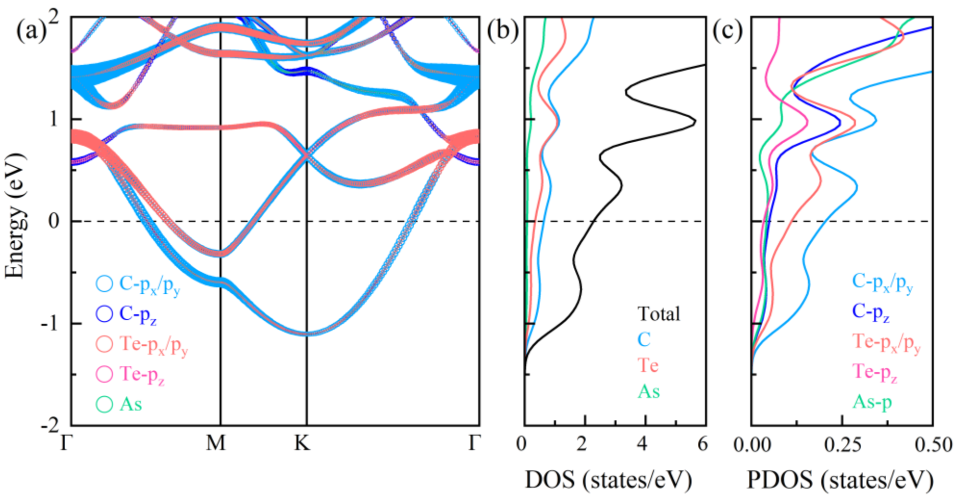

Fig. S5: Band (a), DOS (b) and PDOS (c) for $AsTeC_3$.

VII. The WCC of $InAsC_3$ $SeAsC_3$ and $InTeC_3$

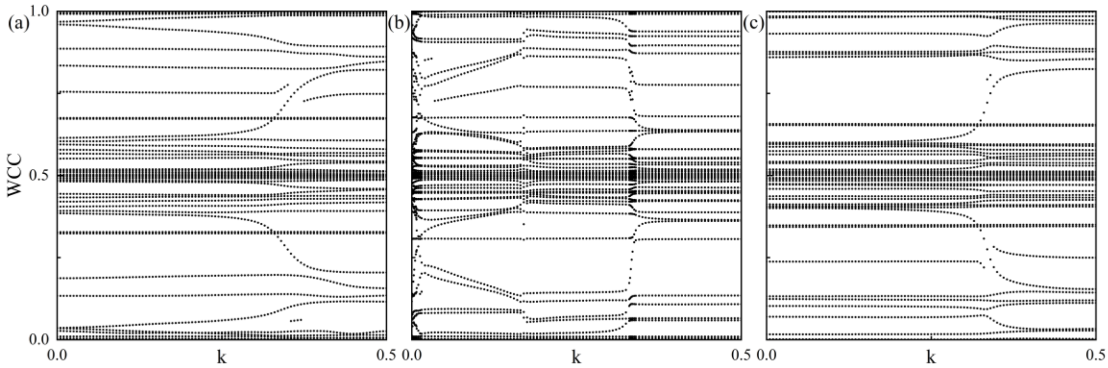

Fig. S6: Evolution of WCC (a) $InAsC_3$, (b) $SeAsC_3$, (c) $InTeC_3$.

VIII. The superconductivity of $AsTeC_3$

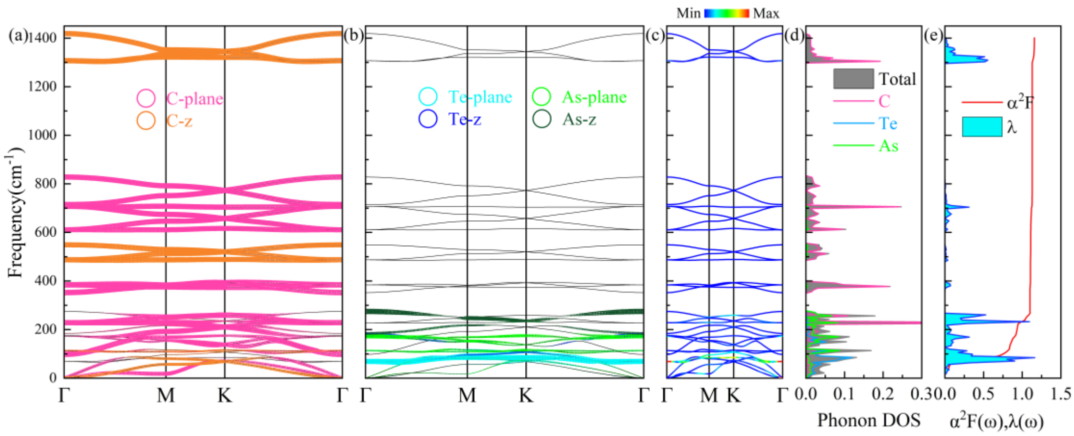

Fig. S7: Phonon dispersion (a,b) weighted by the vibrational modes of C, Te and As atoms, respectively. (c) Phonon dispersion weighted by the magnitude of EPC λ_{qv}. (d) Total and atom-projected phonon DOS. (e) Eliashberg spectral function $\alpha 2F(\omega)$ and cumulative frequency-dependent EPC function $\lambda(\omega)$.

IX. The dynamic stability of $SeAsC_3$ at degauss = 0.04

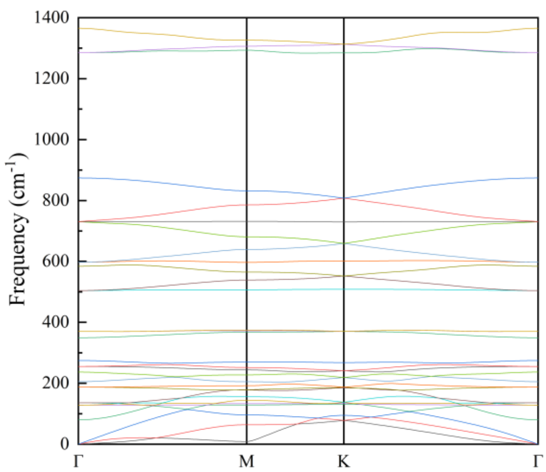

Fig. S8: Phonon spectra of $SeAsC_3$ at degauss = 0.04.

X. The comparison of EPC parameter λ, logarithmic average phonon frequency ω_{log} (K), and superconducting transition temperatures T_c (K) corresponding to different materials.

	λ	ω_{log} (K)	T_c (K)
$InAsC_3$	2.57	134	33.632
$SeAsC_3$	1.09	209	16.645
$InTeC_3$	0.48	222	2.401
$AsTeC_3$	1.16	153	13.129

Table S1. The calculated EPC parameter λ, logarithmic average phonon frequency ω_{log} (K), and superconducting transition temperatures T_c (K) corresponding to different materials.

References

1 W. L. McMillan, Phys. Rev., 1968, 167, 331.
2 R. C. Dynes, Solid State Commun., 1972, 10, 615.
3 P. B. Allen and R. C. Dynes, Phys. Rev. B, 1975, 12, 905-922.
4 J. Kortus, et al., Phys. Rev. Lett., 2001, 86, 4656-4659.