Electronic Supplementary Material (ESI) for Nanoscale Horizons.

One Dimensional Ferroelectric Nanothread with both Axial and Radial Polarization

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I. Phonon spectra of ω_3 nanothreads of III_2VI_3

The phonon spectra of ω_3 nanothreads of III_2VI_3 along the high-symmetry path ($\Gamma \rightarrow$ Y) are shown in Fig. S1. For each q point, we calculated the corresponding phonon frequencies with density functional perturbation theory. Here, we did not perform Fourier interpolation. The phonon spectrum of ω_3 nanothread of Ga_2Se_3 has no imaginary vibrational frequencies, confirming its dynamical stability. Ga_2S_3, Ga_2Te_3 and Al_2Te_3 are probably marginally stable as only the lowest acoustic mode has small imaginary frequencies ($< 10i$ cm^{-1}), while all the other nanothreads of Al_2S_3, Al_2Se_3, Ga_2S_3, In_2S_3, In_2Se_3, and In_2Te_3 are all unstable for their large imaginary frequencies near Y.

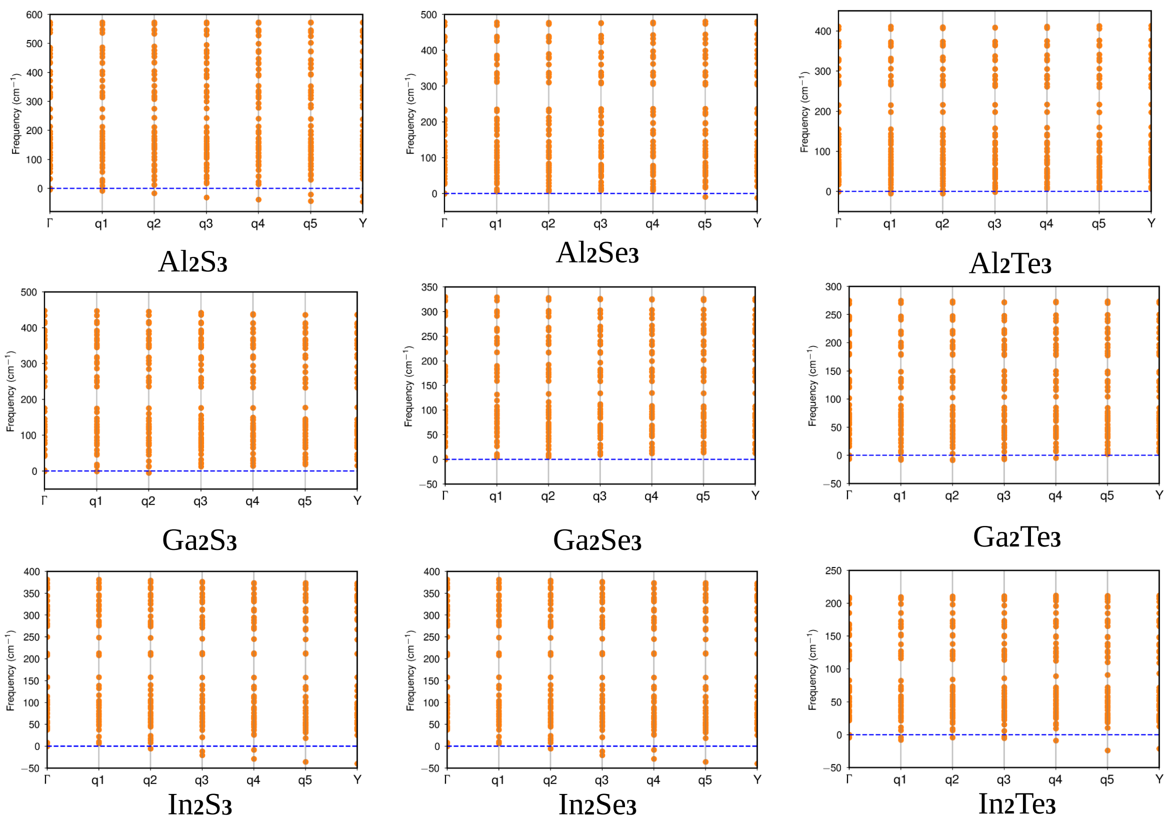

Figure S1: Phonon spectra of ω_3 nanothreads of III_2VI_3 (III=Al, Ga, In; VI=S, Se, Te).

II. Packed ω_3 nanothreads

To estimate the density of packed ω_3 nanothreads, we constructed a cell containing four aligned ω_3 Ga_2Se_3 nanothreads along the b axis (Fig. S2) and fully optimized both the atomic positions and cell dimensions. The equilibrium distance between nanothreads in the optimized cell is ≈3.5 Å. The calculated van der Waals (vdW) binding energy is ≈0.4 eV/Å, corresponding to a vdW binding energy of ≈60 meV/Å^2. This value is comparable to the vdW binding energy in many layered vdW materials (e.g., 25∼30 meV/Å^2 for layered compounds of transition metal dichalcogenides.[1]) The averaged lattice constants of one single nanothread in a crystal is $\bar{a}$ = 9.725 Å , $\bar{b}$ = 6.158 Å, and $\bar{c}$ = 9.251 Å. Assuming a 1D domain of 3 unit cells being the minimum storage unit, the theoretical data density for an atomically thin layer of 1DFENT array in the yz plane is $1\text{bit}/3\bar{b}\bar{c} \approx 600$ Gb/mm^2. Furthermore, by packing 1DFENTs into 3D arrays, the upper bound of the volumetric density could approach $1\text{bit}/3\bar{a}\bar{b}\bar{c} \approx 600$ Petabit/mm^3.

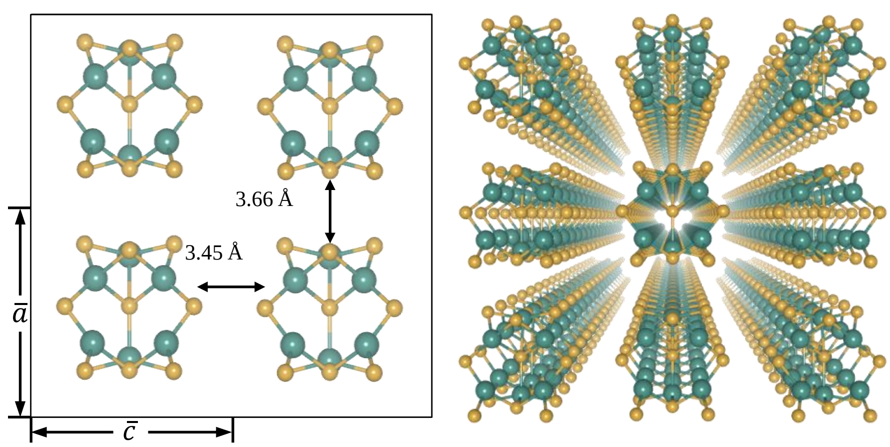

Figure S2: DFT optimized cell containing four parallel ω_3 nanothreads.

III. ω_3 nanothreads on graphene

We designed a model in which graphene serves as a 2D substrate to support an ω_3 nanothread of Ga_2Se_3. The atomic positions in this model have been fully optimized with DFT. As shown in Fig. S3, the gap between the ferroelectric nanothread and the graphene is 3.5 Å, a typical vdW distance.

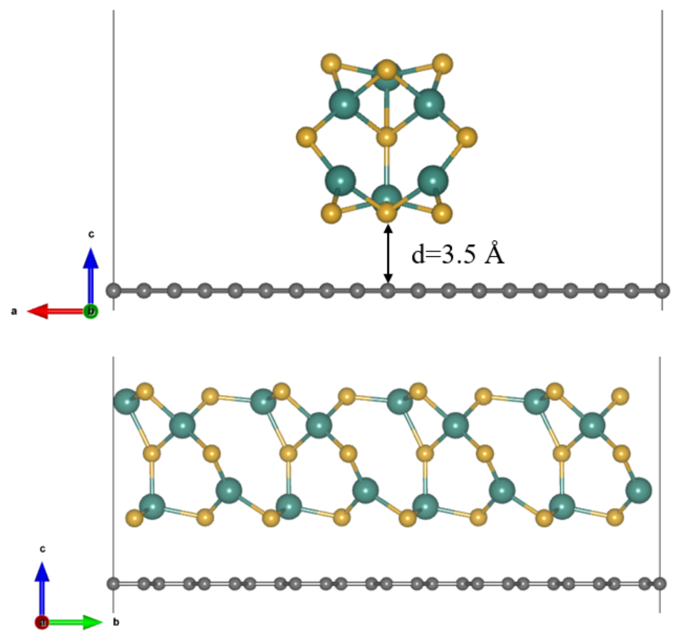

Figure S3: DFT optimized ω_3 nanothreads supported by graphene.

IV. Raman spectrum of ω_3 nanothreads

We calculated the Raman spectrum of ω_3 nanothread of Ga_2Se_3 (Fig. S4), which could be helpful for experimental characterizations of nanothreads.

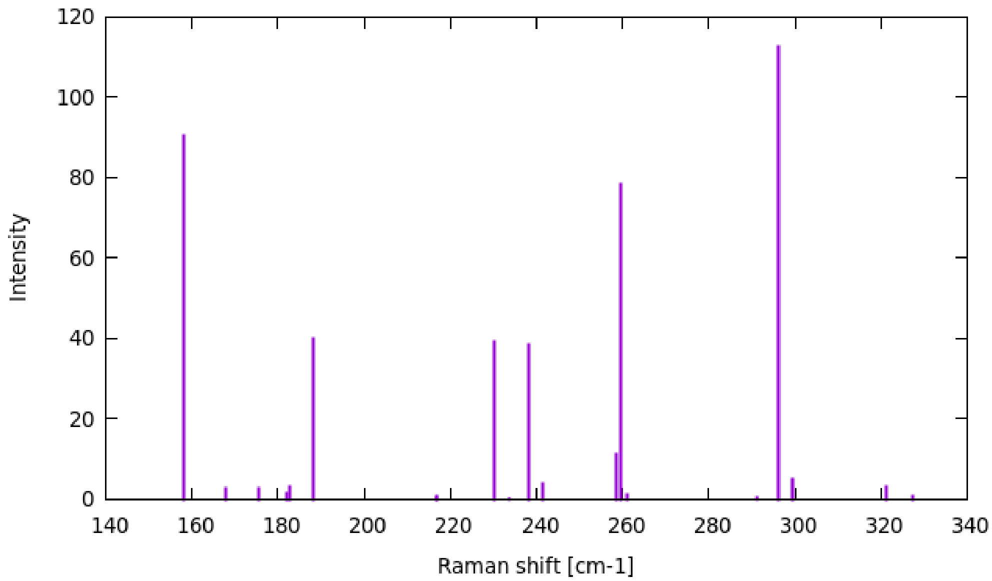

Figure S4: Raman spectrum of ω_3 nanothread of Ga_2Se_3.

References

(1) Rydberg, H.; Dion, M.; Jacobson, N.; Schröder, E.; Hyldgaard, P.; Simak, S. I.; Langreth, D. C.; Lundqvist, B. I. Van der Waals Density Functional for Layered Structures. *Phys. Rev. Lett.* **2003**, *91*, 126402.