Supplementary Material for

Semimetallic Superconductivity in Cubic Nd_3In: A First-Principles Insight into Indium-Based Compounds

Arafat Rahman, Alamgir Kabir, and Tareq Mahmud

Department of Physics, University of Dhaka, Dhaka 1000, Bangladesh

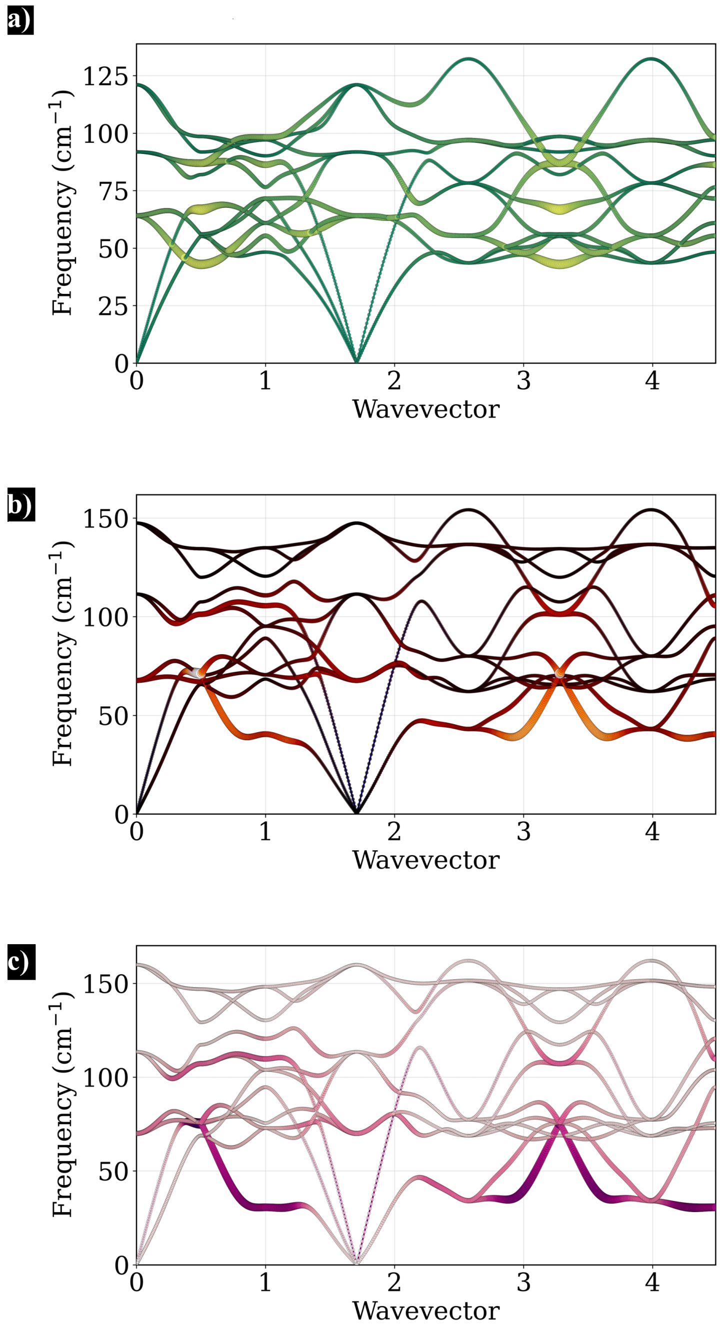

FIG. S1: Phonon dispersion relations of Nd_3In under different hydrostatic pressures. Fat bands indicate modes with strong electron–phonon coupling. (a) At ambient pressure (0 GPa), the phonon spectrum shows distinct acoustic and optical branches. (b) At 10 GPa, acoustic phonon branches soften, reflecting pressure-induced lattice changes. (c) At 15 GPa, further softening is observed in the low-frequency region. The electron-phonon coupling constant λ increases with pressure, suggesting enhanced superconducting interactions.

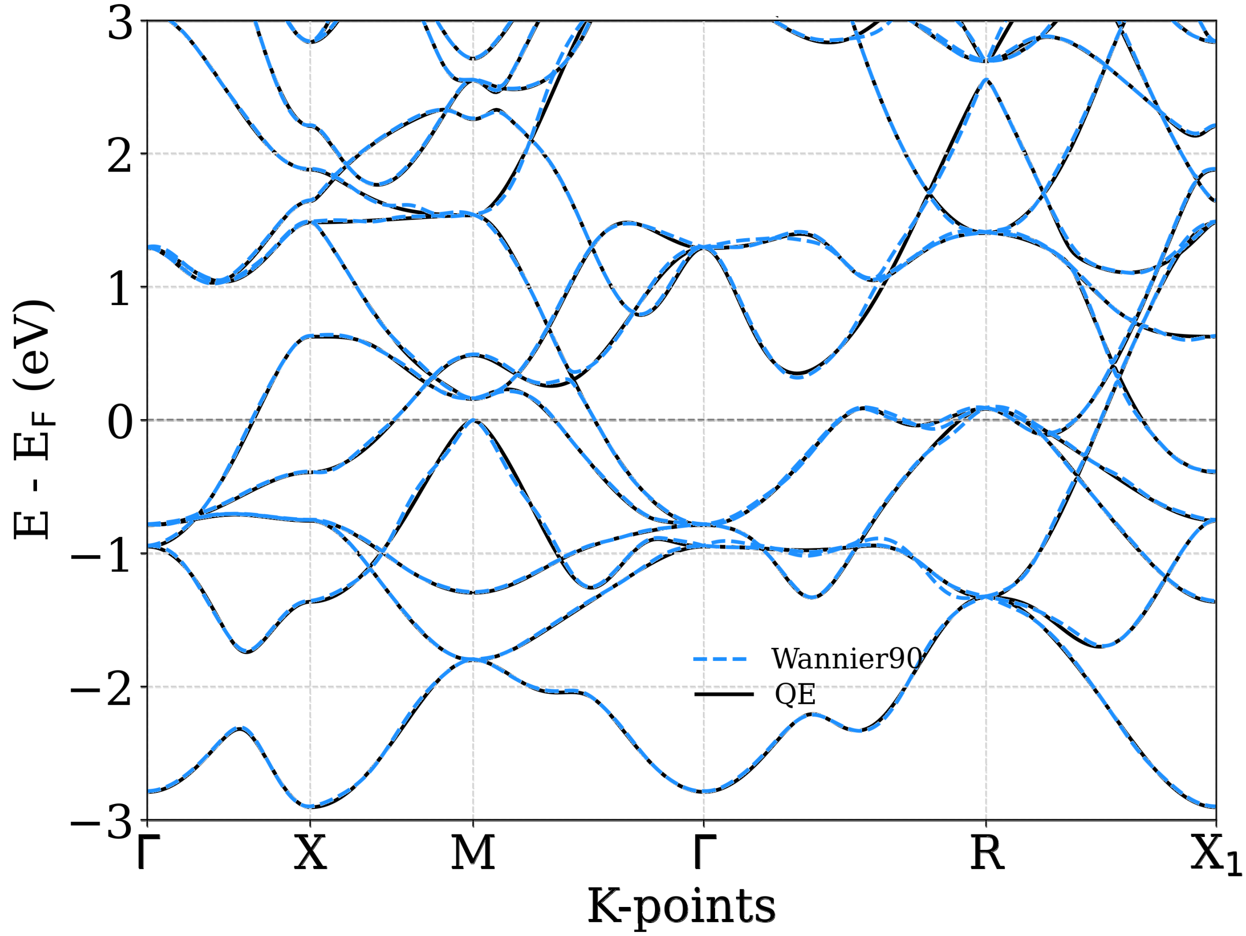

FIG. S2: Electronic band structure of Nd_3In without spin–orbit coupling. The Wannier90-interpolated bands are shown as blue dashed lines; DFT bands as solid black lines.

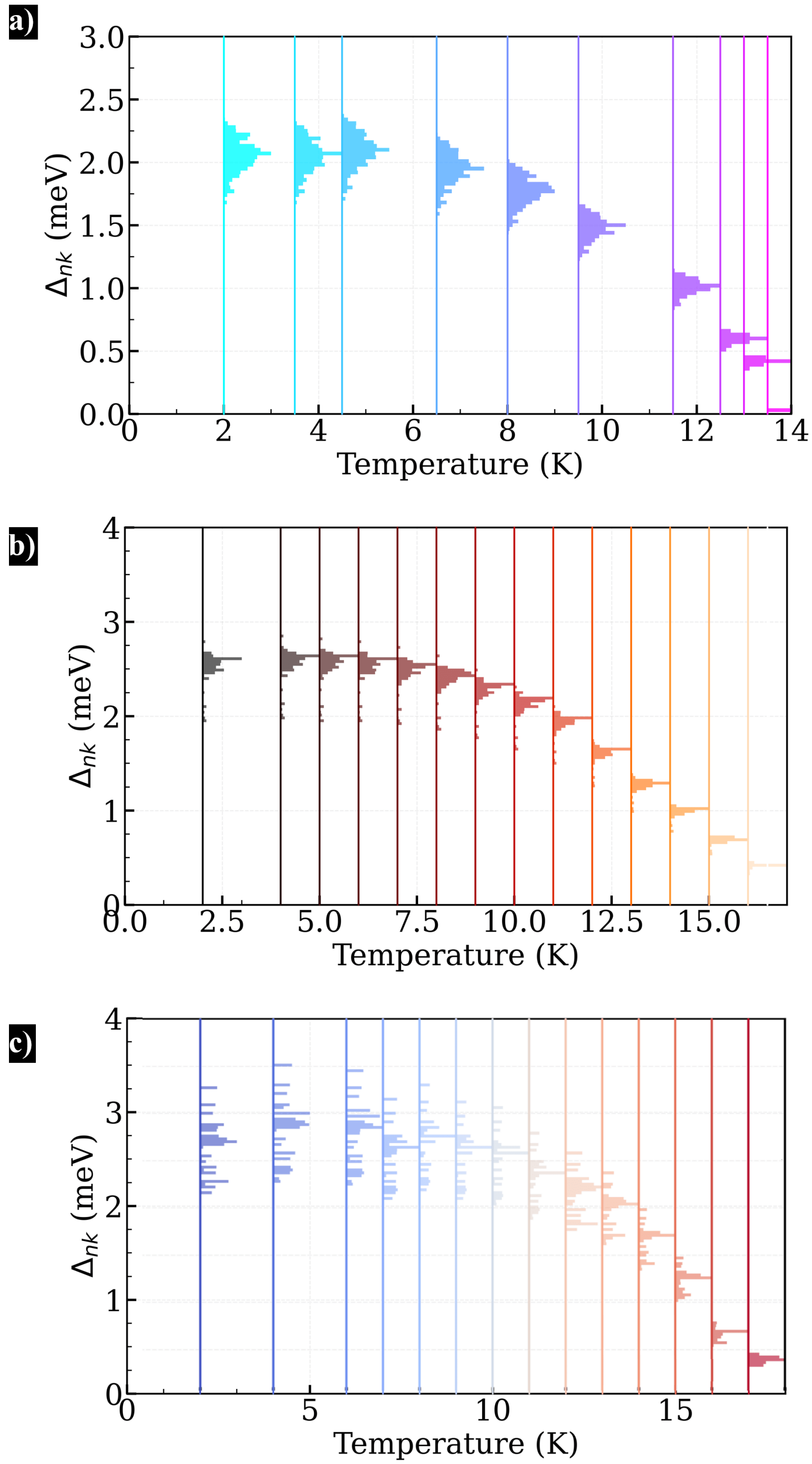

FIG. S3: Temperature dependence of the anisotropic superconducting gap on the Fermi surface of Nd_3In. (a) At 0 GPa, the gap closes near 14 K. (b) At 10 GPa, it persists up to 16.5 K. (c) At 15 GPa, it remains open up to 18 K, confirming pressure-induced enhancement of T_c.

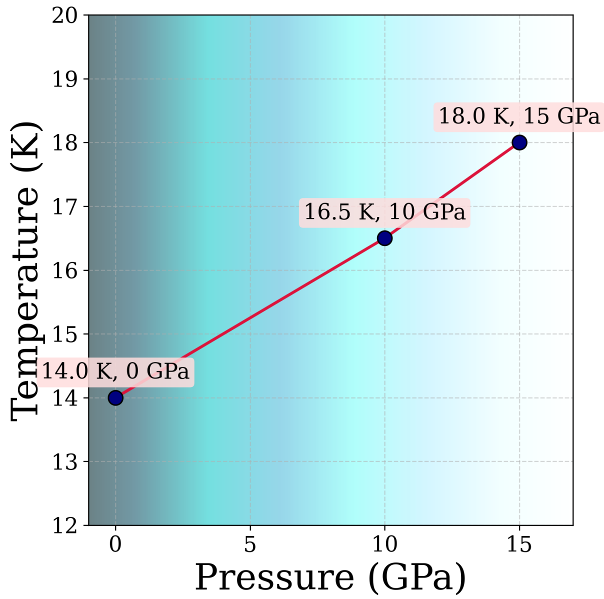

FIG. S4: Superconducting transition temperature T_c of Nd_3In at different pressures (0, 10, and 15 GPa) from anisotropic Eliashberg theory. A clear enhancement of T_c with increasing pressure is observed.

TABLE A1: Total energies of Nd_3In for different magnetic configurations.

Magnetic Config.	**Total Energy (Ry)**	**Total Magnetization** (μ_B	ΔE w.r.t NM (Ry)	ΔE w.r.t NM (eV)
Nonmagnetic (NM)	-521.37877592	0.00	0.00000	0.0000
Antiferromagnetic	-521.37823121	0.00	+0.00054471	+0.0074
Ferromagnetic (FM)	-521.00284678	9.00	+0.37592914	+5.11

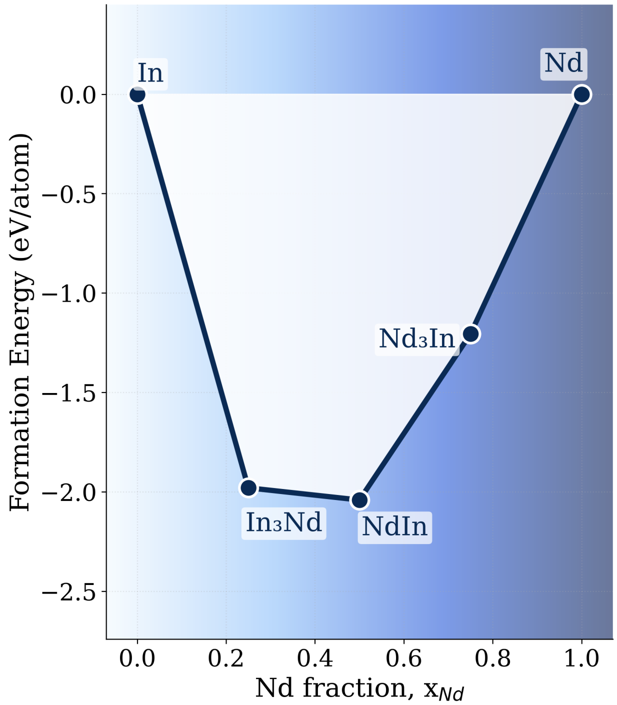

FIG. S5: Convex hull of the Nd–In binary system showing the stability of In_3Nd and Nd_3In.

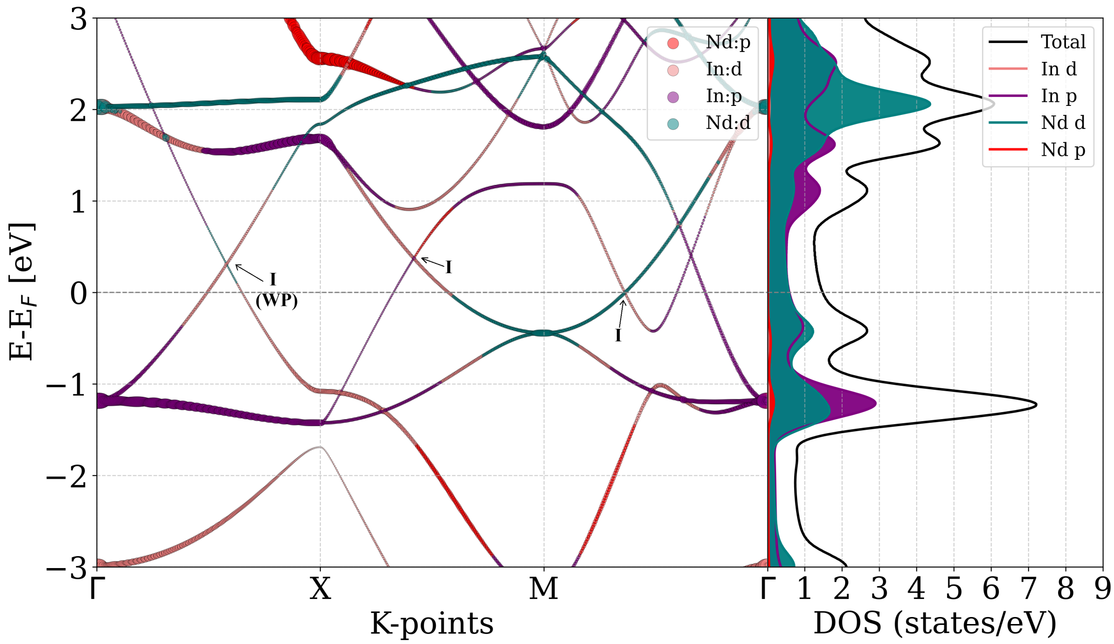

FIG. S6: Orbital-projected band structure and density of states (PDOS) for In_3Nd without spin–orbit coupling. Scatter size indicates orbital contribution. The total DOS at the Fermi level is 1.51 states/eV, indicating limited electronic states.

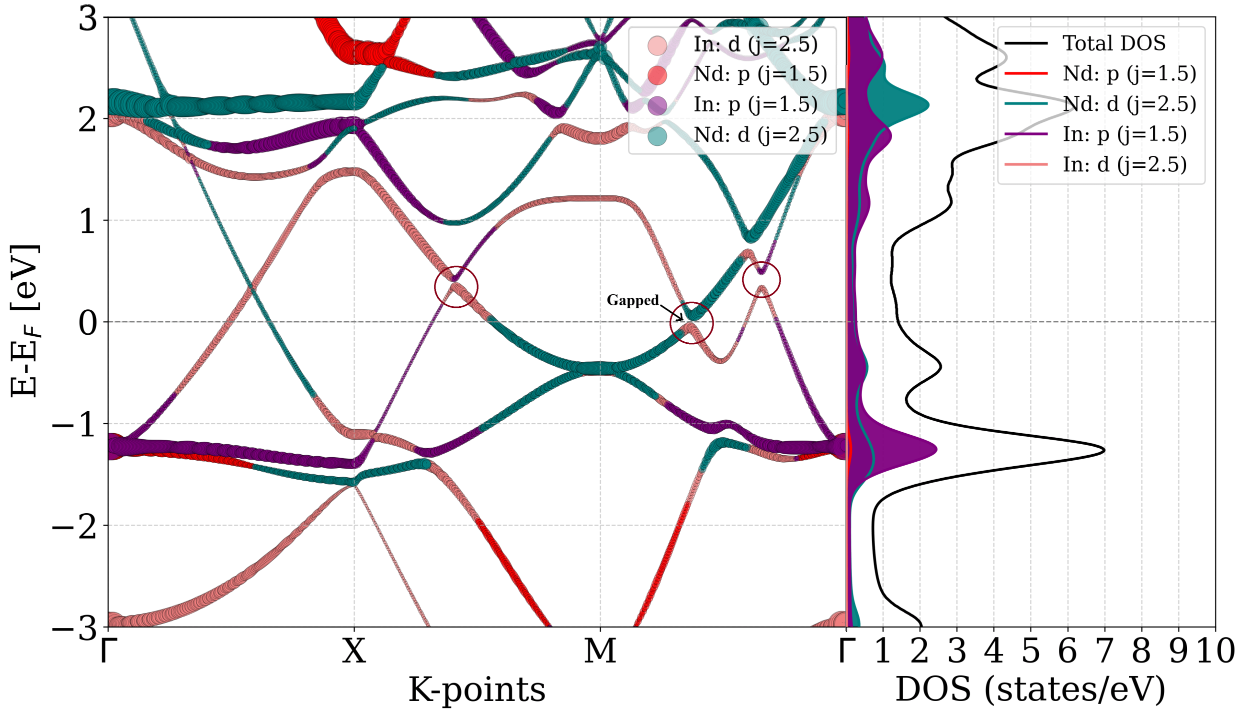

FIG. S7: Band structure and PDOS of In_3Nd with spin–orbit coupling. Orbital projections shown by scatter size. DOS at the Fermi level slightly decreases to 1.38 states/eV. Several band gaps appear due to SOC.

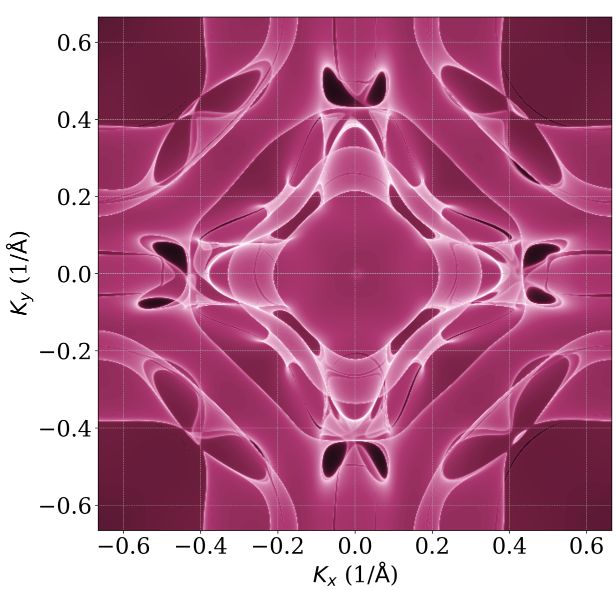

FIG. S8: Fermi arcs in In_3Nd, indicating semimetallic character.

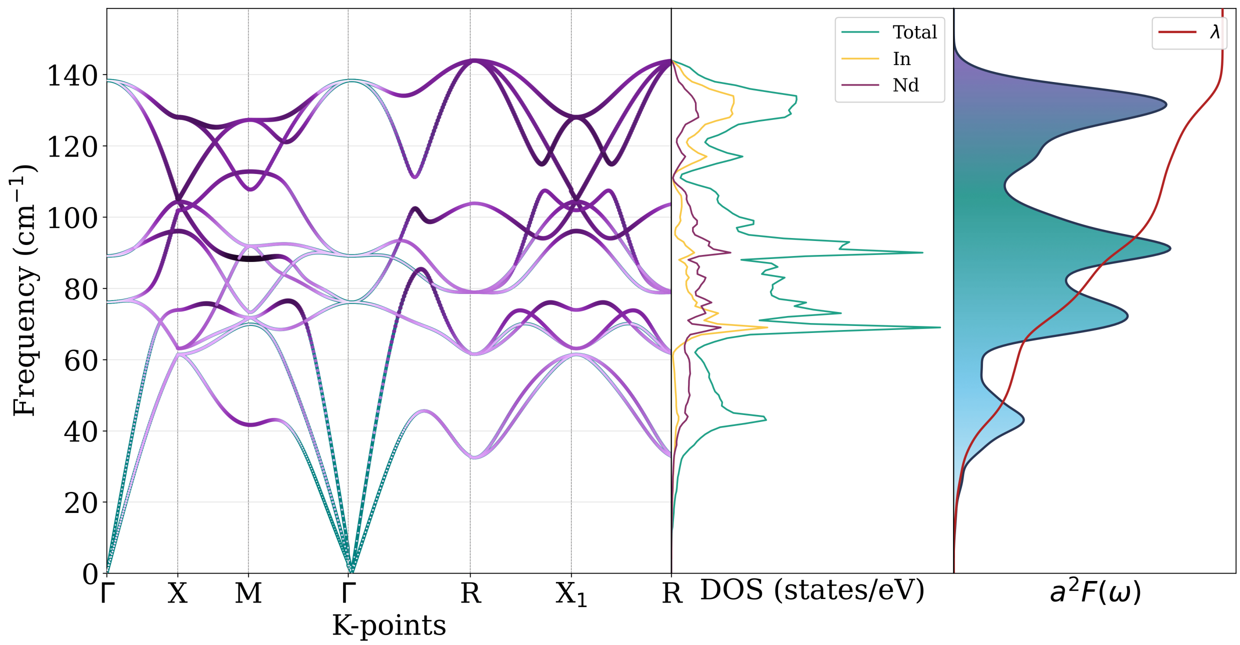

FIG. S9: Phononic and superconducting properties of In_3Nd. Left: phonon dispersion weighted by mode-resolved EPC $\lambda_{\mathbf{q}\nu}$. Middle: atom-projected phonon DOS. Right: Eliashberg spectral function $\alpha^2F(\omega)$ and integrated EPC $\lambda(\omega)$.