

Grokrone v2: An Audit of the Original Grokrone Prediction and a First-Principles Reassessment Based on Hole-Doped Graphane

PROJECT 486 Labs

Correspondence: ben@project486.org

October 2026

Abstract

We revisit *Grokrone*, a potassium-intercalated graphene superlattice previously proposed as a room-temperature, ambient-pressure superconductor candidate (arXiv:2601.00931, “v1”). An internal audit shows that the reported electron-phonon parameters of v1 are not mutually consistent. The logarithmic phonon frequency $\omega_{\log} \approx 1650$ K can’t be reconciled with an Eliashberg function whose coupling is dominated by modes below ~ 400 cm⁻¹. The quoted gap ratio $2\Delta/k_B T_c = 3.4$ is incompatible with $\lambda = 3.8$. The quoted Berezinskii-Kosterlitz-Thouless temperature does not follow from the stated superfluid density. We therefore withdraw the v1 numerical claims. We replace them with a fully reproducible calculation on a physically better-motivated member of the same graphene family: chair graphane (C₂H₂) with hole doping, in which metallized C–C σ bonds couple to stiff bond-stretching phonons, the mechanism of MgB₂. Using density-functional perturbation theory and Wannier-interpolated Migdal-Eliashberg theory, we find that 3–7% hole doping ($1.1\text{--}2.6 \times 10^{14}$ cm⁻²) gives isotropic Eliashberg critical temperatures of 50–71 K ($\mu^* = 0.13$). T_c saturates towards the top of this range. These are above the MgB₂ record for conventional superconductors at ambient pressure but far below room temperature. The coupling is carried by the Raman-active E_g C–C stretching mode, which softens from 1102 to 764 cm⁻¹ on doping. Phase fluctuations do not limit T_c in clean monolayers. We discuss multilayer routes and the experimental signatures that would confirm or falsify the prediction. All inputs, outputs and scripts are released.

1 Introduction

Conventional (phonon-mediated) superconductivity at ambient pressure currently tops out experimentally at 39 K in MgB₂ [1]. A recent high-throughput study of more than 2×10^4 metals finds that the trade-off between the coupling strength λ and the characteristic phonon frequency $\omega_{\log}$ makes room-temperature conventional superconductivity at ambient pressure “extremely unlikely”, with the best computed candidates near 100 K [2]. Any claim beyond that envelope therefore carries a heavy burden of internal consistency.

The first Grokrone report (v1) [3] claimed $\lambda \approx 3.8$ together with $\omega_{\log} \approx 1650$ K for an alkali-intercalated graphene superlattice. Section 2 shows that this combination is not supported by the paper’s own spectral data. Section 3 then moves to hole-doped graphane. Savini, Ferrari and Giustino predicted this system to superconduct above 90 K [4], and it is the most credible graphene-derived route to high- T_c conventional superconductivity in the literature. Here we recompute its properties from scratch with an open, reproducible workflow.

2 Audit of the v1 prediction

All numbers below use only quantities printed in v1.

(i) **$\omega_{\log}$ versus the Eliashberg function.** By definition $\omega_{\log} = \exp[\frac{2}{\lambda} \int \frac{d\omega}{\omega} \alpha^2 F(\omega) \ln \omega]$, i.e. the λ -weighted geometric mean of the phonon frequencies. v1 states that coupling is dominated by dopant modes at 110–150 cm^{-1} and modes up to $\sim 400 \text{ cm}^{-1}$ (v1, Fig. 3), with a smaller contribution from the E_{2g} branch near 1580 cm^{-1} . A two-channel estimate shows that $\omega_{\log} = 1650 \text{ K}$ requires $\approx 87\%$ of λ to come from the 1580 cm^{-1} channel. If instead 60% of λ comes from the 130 cm^{-1} channel, $\omega_{\log} \approx 510 \text{ K}$ and the Allen–Dynes T_c falls to 100–150 K (with or without the $f_1 f_2$ strong-coupling factors).

(ii) **Strong-coupling gap ratio.** For $T_c/\omega_{\log} = 0.19$ the standard strong-coupling correlation $2\Delta/k_B T_c \simeq 3.53[1 + 12.5(T_c/\omega_{\log})^2 \ln(\omega_{\log}/2T_c)]$ gives ≈ 5.0 . v1 reports 3.4, a weak-coupling value, from $\Delta(0) = 45 \text{ meV}$ and $T_c = 310 \text{ K}$.

(iii) **Allen–Dynes arithmetic.** v1 quotes $T_c^{\text{MF}} = 325 \text{ K}$ from the bare Allen–Dynes expression. Including the $f_1 f_2$ corrections that are mandatory at $\lambda \approx 3.8$ gives $\approx 485 \text{ K}$. That would contradict the Eliashberg value of 310 K by a far larger margin than the stated vertex-correction estimate.

(iv) **BKT temperature.** With the v1 inputs $n_s^{2D} = 3.5 \times 10^{13} \text{ cm}^{-2}$ and $m^* = 1.3m_e$, the quoted formula gives $T_{\text{BKT}} \approx 94 \text{ K}$, not 120 K. v1 Fig. 5 places the crossing near 60 K.

(v) **Methods and structure.** v1 attributes DFPT/EPW calculations to GPAW, whereas EPW is part of Quantum ESPRESSO. A hexagonal cell is reported with $a = 9.84 \text{ \AA}$ and $b = 8.52 \text{ \AA}$ ($= a \cos 30^\circ$). The space group is given as “P6/m2”, which is not a valid symbol.

Given (i)–(v), we regard the v1 values of λ , $\omega_{\log}$ and T_c as unsupported.

3 Groke v2: hole-doped graphane

3.1 Rationale

Graphane is graphene fully hydrogenated on alternating sides. All carbons are sp^3 and the material is an insulator with a σ -bonded valence band [5, 6]. Removing electrons from that band metallizes C–C σ bonds. This is the same ingredient that drives superconductivity in MgB_2 and boron-doped diamond, but with lighter atoms and stiffer bonds. The resulting coupling is moderate ($\lambda \sim 1$) but sits on a high frequency scale. This is precisely the regime in which a high $\omega_{\log}$ is physically legitimate, unlike v1.

3.2 Computational details

Calculations use Quantum ESPRESSO [7, 8] within the local-density approximation, with norm-conserving pseudopotentials (C: FHI/Troullier–Martins; H: von Barth–Car) and a 70 Ry plane-wave cutoff. The slab period is 15.1 $\text{\AA}$. The in-plane lattice and internal coordinates are relaxed at zero doping ($18 \times 18 \times 1$ k -mesh, residual forces $< 10^{-4} \text{ Ry/bohr}$).

Hole doping x (holes per C) is introduced by removing $2x$ electrons per cell with a compensating uniform background. We consider $x = 1\%$, 3% and 5% , i.e. $n_h \approx 0.37$, 1.1 and $1.9 \times 10^{14} \text{ cm}^{-2}$. Phonons and electron–phonon matrix elements are computed by DFPT on a $6 \times 6 \times 1$ q -mesh ($24 \times 24 \times 1$ k -mesh, Marzari–Vanderbilt smearing 0.02 Ry). They are Wannier-interpolated with EPW [9] onto fine meshes of up to 300×300 k and 150×150 q points (Sec. 3, convergence). For $x = 5\%$ the coarse DFPT k -mesh is 18×18 , which changes test phonon frequencies by less than 2% relative to 24×24 . Five bond-centred Wannier functions (three C–C, two C–H) span the isolated valence manifold. The isotropic Migdal–Eliashberg equations are solved on the imaginary axis with $\mu^* = 0.13$ (following Ref. [4]) and continued to the real axis by Padé approximants.

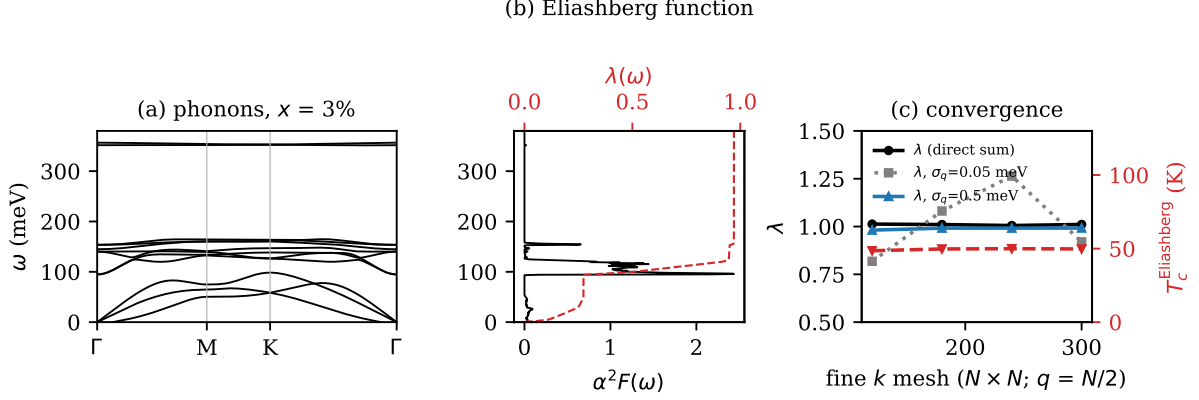


Figure 1: Hole-doped graphane, $x = 3\%$. (a) Phonon dispersion, Fourier-interpolated from the 6×6 DFPT mesh. (b) Isotropic Eliashberg function and cumulative $\lambda(\omega)$. (c) Convergence of λ and T_c with the fine Wannier mesh. The direct Fermi-surface sum of λ (black) and the α^2F integral with 0.5 meV phonon smearing (blue) are converged to ± 0.01 . A 0.05 meV phonon smearing (grey) gives spurious grid-to-grid scatter in λ between 0.8 and 1.3.

3.3 Structure

The relaxed structure has $a = 2.494$ Å, $d_{\text{C-C}} = 1.51$ Å, $d_{\text{C-H}} = 1.11$ Å, and a C buckling of ± 0.22 Å. The undoped sheet is a direct-gap insulator with an LDA gap of 3.36 eV at Γ , consistent with earlier semilocal calculations [5]. The valence-band maximum is a doubly degenerate σ state of C-C bonding character.

3.4 Electronic structure under hole doping

Removing $2x$ electrons per cell creates two concentric hole pockets around Γ , one light and one heavy. At $x = 3\%$ the Fermi level lies 0.288 eV below the VBM. Effective masses are $m^* = 0.28 m_e$ and $0.62 m_e$, with $k_F = 0.145$ and 0.218 Å $^{-1}$. The two pockets hold 3.4×10^{13} and 7.6×10^{13} cm $^{-2}$ holes, which sum to the imposed $n_h = 1.1 \times 10^{14}$ cm $^{-2}$. The density of states at E_F is $N(E_F) = 0.110$ states/eV/spin/cell, in agreement with Ref. [4] (0.22 states/eV/cell including spin). Five bond-centred Wannier functions reproduce the DFT valence bands. Their spreads are 0.73 Å (C-C) and 0.77 Å (C-H).

3.5 Phonons and electron-phonon coupling

All seven irreducible DFPT q -points at $x = 3\%$ are dynamically stable. The lowest computed frequency at finite q is 66 cm $^{-1}$. After Fourier interpolation, the flexural (ZA) branch shows small negative values (≥ -9 cm $^{-1}$) close to Γ . This is the usual interpolation artefact for flexural modes without rotational sum rules, and it does not appear at any explicitly computed q -point.

Doping has a dramatic effect on the Raman-active in-plane C-C stretching mode. The E_g mode at Γ softens from 1102 cm $^{-1}$ in the undoped sheet to 764 cm $^{-1}$ at $x = 3\%$ (-338 cm $^{-1}$, -42 meV). The other Γ modes shift by less than 30 cm $^{-1}$, and the C-H stretching modes (2834–2876 cm $^{-1}$) do not move. In the E_g eigenvector the hydrogen displacements are 2.6 times larger than the carbon ones, so the mode is a coupled C-C stretch and C-H bend.

The Eliashberg function (Fig. 1b) is dominated by this branch near Γ . Of the total λ , about 0.7 comes from modes between 90 and 125 meV and about 0.25 from acoustic modes below 40 meV. The C-H stretching region contributes nothing.

Convergence. Because the hole pockets are small, λ comes mainly from intra-pocket scattering with $q < 2k_F \approx 0.4 \text{ \AA}^{-1}$, and the result is sensitive to Brillouin-zone sampling. We varied the fine mesh from 120×120 to 300×300 in k , with half as many points in q . The direct sum of λ over the Fermi surface is converged to 1.01 ± 0.01 for all meshes (Fig. 1c). The $\alpha^2 F$ histogram, however, is noisy if the phonon smearing is too small (0.05 meV), and then its integral scatters between 0.8 and 1.3. Isotropic Eliashberg solutions based on that histogram scatter between 18 and 87 K. With a 0.5 meV phonon smearing every mesh from 180×180 upward gives the same $\alpha^2 F$ to within 1%. We use the $300 \times 300 / 150 \times 150$ result. Halving the electronic smearing from 50 to 25 meV changes λ by 4%. We note this explicitly because the scattered values are exactly the kind of number that, quoted without a convergence study, produced the v1 claims.

3.6 Superconducting properties

Table 1: Superconducting parameters of hole-doped graphane. λ_{tot} is the direct Fermi-surface sum. $\lambda_{>5}$, ω_{log} and T_c^{AD} use the Eliashberg function with $\omega > 5$ meV, which removes the interpolation-sensitive flexural region near Γ ; T_c^{El} is insensitive to this choice (within 1 K). T_c values use $\mu^* = 0.13$, with the range for $\mu^* = 0.10$ – 0.16 in brackets. Δ_0 is the gap at the first Matsubara frequency at 5 K.

x	$n_h \text{ (cm}^{-2}\text{)}$	$N(E_F)$	λ_{tot}	$\lambda_{>5}$	$\omega_{\text{log}} \text{ (K)}$	$T_c^{\text{AD}} \text{ (K)}$	$T_c^{\text{El}} \text{ (K)}$	$\Delta_0 \text{ (meV)}$	$\frac{2\Delta_0}{k_B T_c}$
3%	1.1×10^{14}	0.110	1.01	0.86	870	41 [33–50]	50 [44–57]	8.2	3.8
5%	1.9×10^{14}	0.114	1.28	1.12	660	52 [44–59]	63 [57–70]	10.8	4.0
7%	2.6×10^{14}	0.120	2.05	1.36	540	56 [49–63]	71 [65–78]	12.6	4.1

At $x = 3\%$ we obtain $\lambda_{\text{tot}} = 1.01$, of which 0.86 comes from modes above 5 meV, with $\omega_{\text{log}} = 870$ K for that part. Allen–Dynes (with $f_1 f_2$) gives $T_c = 41$ K. The isotropic Eliashberg equations, solved independently with EPW and with our own Matsubara-axis solver, give $T_c = 50$ K. In the EPW solution the gap closes between 45 and 55 K. Our linearized solver gives 49.8 K, and both give the same $\Delta_0 = 8.16$ meV at 5 K. The gap ratio $2\Delta_0/k_B T_c = 3.8$ is consistent with the coupling strength. For $T_c/\omega_{\text{log}} = 0.057$ the strong-coupling correlation predicts 3.84. Unlike v1 (Sec. 2), every quantity in the table follows from the same $\alpha^2 F$.

At $x = 5\%$ the coupling increases to $\lambda_{\text{tot}} = 1.28$. Here the direct sum and the $\alpha^2 F$ integral agree for every phonon smearing, because the larger pockets are easier to sample. T_c^{El} rises to 63 K, and the EPW gap is still 4.1 meV at 60 K. $\Delta_0 = 10.8$ meV is reproduced by both solvers. The Γ -point E_g mode is at 746 cm^{-1} . The contribution of acoustic modes below 40 meV grows from 0.25 to 0.48. These modes change λ and ω_{log} but barely change T_c : removing all spectral weight below 20 meV lowers T_c by only 2 K at both dopings. We therefore regard T_c as the robust output and λ , ω_{log} as partly convention-dependent.

At $x = 7\%$ ($2.6 \times 10^{14} \text{ cm}^{-2}$), T_c continues to rise but more slowly, reaching 71 K (Fig. 2a). EPW and our solver again agree: the EPW gap is 2.3 meV at 70 K and closed at 80 K, and both give $\Delta_0 = 12.6$ meV. Two features suggest that the useful doping window ends near this point. First, the softening of the Γ -point E_g mode is largest at 5% and partly reverses at 7% (Fig. 2c), because the region of strong intra-pocket coupling moves to finite q as $2k_F$ grows. Second, low-frequency acoustic spectral weight grows quickly, and the interpolated flexural branch reaches -19 cm^{-1} near Γ . An explicit DFPT calculation at $q = |\mathbf{b}|/12$ ($0.13 \text{ \AA}^{-1}$) gives a ZA frequency of -20 cm^{-1} at 7%, compared with -2.5 cm^{-1} at 3% for identical numerical settings. Long-wavelength flexural frequencies are notoriously sensitive to numerical parameters, so the absolute values are not significant. The doping-induced softening of $\sim 18 \text{ cm}^{-1}$ is. A tendency towards rippling at high doping therefore cannot be excluded for a free-standing sheet. A substrate or encapsulation would suppress it. This region does not affect T_c , which changes by at most 3 K when all spectral weight below 20 meV is removed. Higher densities are also beyond what electrolyte

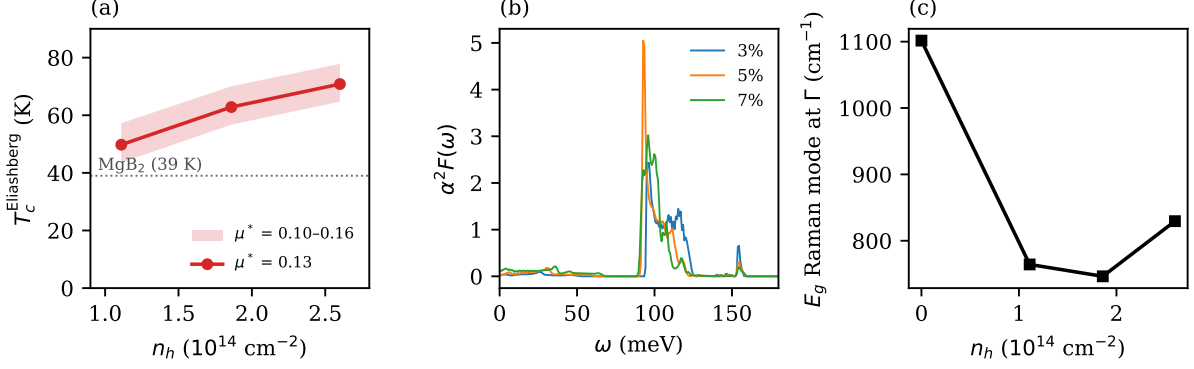


Figure 2: Doping dependence. (a) Isotropic Eliashberg T_c against hole density. The band shows $\mu^* = 0.10-0.16$, and the dotted line marks the MgB_2 record. (b) Eliashberg functions at 3, 5 and 7% (phonon smearing 0.5 meV). (c) Frequency of the Raman-active E_g mode at Γ .

gating has demonstrated in graphene [10]. We therefore regard $T_c \approx 70$ K as a practical ceiling for monolayer hole-doped graphane within this model.

Comparison with Ref. [4]. Savini *et al.* predicted T_c above 90 K for p-doped graphane. Our values are 20–45% lower at comparable doping. Our calculation does not resolve the origin of the difference. Both studies use $\mu^* = 0.13$. Plausible sources of the difference are the doping model, the lattice parameter, and Brillouin-zone sampling. Ref. [4] uses a rigid-band approximation, whereas here the doped charge density, phonons and matrix elements are all computed self-consistently. We stress that hole-doped graphane is *their* proposal. The present work contributes an independent, openly reproducible re-evaluation with a documented convergence study, the doping dependence, the BKT analysis and specific spectroscopic tests.

4 Two-dimensional phase fluctuations

In a single sheet the observable transition is the BKT temperature, set by the superfluid stiffness. For a clean BCS-like superconductor with Fermi-surface carrier density n and mass m^* , $k_B T_{\text{BKT}} \leq \pi \hbar^2 n_s / (8m^*)$. With two pockets the bound becomes $\pi \hbar^2 \sum_i n_i / m_i^* / (8k_B)$. Using the computed masses and pocket densities, the clean-limit bound at $x = 3\%$ is ≈ 850 K. This is far above T_c , so in clean samples phase fluctuations are not the limiting factor. In the dirty limit the superfluid density drops roughly by $\Delta / (\hbar \tau)$, and BKT suppression becomes relevant only for very short scattering times. Hole-doped graphane therefore does not suffer from the $T_{\text{BKT}} \ll T_c$ problem that the v1 analysis itself identified. Multilayer graphane [11] or hBN-encapsulated stacks restore three-dimensional coherence once the interlayer Josephson coupling exceeds the BKT scale.

5 Experimental realization and falsifiable signatures

The prediction requires hole densities of order 10^{14} cm^{-2} in a fully hydrogenated, chair-ordered sheet. Three routes are conceivable. (1) Electrolyte or ionic-liquid gating has reached $\sim 4 \times 10^{14} \text{ cm}^{-2}$ in graphene [10]. It is reversible and lets one scan T_c against n_h on a single device. (2) Substitutional boron, as suggested in Ref. [4], gives permanent doping but introduces disorder and local strain. These are not captured by our uniform-background model. (3) Molecular acceptors are simpler to apply but are unlikely to reach the required density. A separate obstacle is material quality. Graphane obtained by hydrogen-plasma exposure [6] is partially and

inhomogeneously hydrogenated, and dehydrogenates on annealing. Unhydrogenated regions are semimetallic graphene patches that do not share the σ -band mechanism.

The mechanism makes predictions that can be checked independently of a resistive transition:

1. **Phonon softening.** Hole doping softens the Raman-active E_g mode from 1102 to 764 cm^{-1} at $x = 3\%$. This is measurable by Raman spectroscopy under gating, before any superconductivity is sought. Absence of this softening would falsify the model.
2. **Isotope effect.** Most of λ comes from the E_g branch, in which hydrogen co-moves with carbon. Both $^{12}\text{C} \rightarrow ^{13}\text{C}$ and $\text{H} \rightarrow \text{D}$ substitution should therefore give sizeable, measurable isotope shifts. The C–H stretching modes, which do not couple, should not. Quantifying the partial isotope coefficients is left to future work.
3. **Gap ratio.** $2\Delta_0/k_B T_c \approx 3.8$ and $\Delta_0 \approx 8 \text{ meV}$ at $x = 3\%$, measurable by tunnelling.

6 Limitations

The present results should be read with the following limitations. (i) Doping is modelled by removing electrons against a uniform compensating background, which neglects dopant disorder and gate fields. (ii) We solve the isotropic Eliashberg equations. Anisotropy over the small hole pockets is expected to raise T_c modestly, as in MgB_2 , so the isotropic value is closer to a lower estimate. (iii) T_c depends on the Coulomb pseudopotential, and we report its sensitivity for $\mu^* \in [0.10, 0.16]$. (iv) Phonons are harmonic. Anharmonicity of the light C–H modes is neglected, although these modes contribute little to λ (Fig. 1b). (v) The coarse DFPT mesh is 6×6 in q . Kohn anomalies at $2k_F$ are captured only through Wannier interpolation. (vi) LDA slightly underestimates the lattice constant, and λ for σ -band metals is known to be sensitive to strain.

7 Conclusions

The original Groke claims of $\lambda \approx 3.8$, $\omega_{\log} \approx 1650 \text{ K}$ and $T_c \approx 310 \text{ K}$ are not internally consistent and should not be cited as a room-temperature prediction. Recomputing a related graphene-derived system from first principles, with a documented convergence study, gives a smaller and verifiable result. Hole-doped graphane is a dynamically stable, σ -band electron–phonon superconductor. Its predicted T_c is 50–71 K at $n_h = 1.1\text{--}2.6 \times 10^{14} \text{ cm}^{-2}$ (44–78 K for $\mu^* = 0.10\text{--}0.16$), and it saturates near the top of this range. This would be the highest T_c of any conventional ambient-pressure superconductor if confirmed. It is well inside the $\sim 100 \text{ K}$ envelope expected for such materials [2], not at room temperature.

The most direct test does not need a superconducting measurement. Raman spectroscopy of electrolyte-gated graphane should show the E_g mode moving from ~ 1100 to $\sim 760 \text{ cm}^{-1}$ as n_h approaches 10^{14} cm^{-2} . If that softening is absent, the mechanism, and with it this prediction, is ruled out.

Data availability

All inputs, outputs and analysis scripts are available at <https://github.com/project486-labs/groke-v2>.

References

- [1] J. Nagamatsu *et al.*, Nature **410**, 63 (2001).

- [2] K. Gao, T. Cerqueira, A. Sanna, Y.-W. Fang, Đ. Dangić, I. Errea, H.-C. Wang, S. Botti, M. A. L. Marques, Nat. Commun. **16**, 8256 (2025); arXiv:2502.18281.
- [3] DEARDAO DeSci Collaborative Team and Y. Ding, arXiv:2601.00931 (2026).
- [4] G. Savini, A. C. Ferrari, F. Giustino, Phys. Rev. Lett. **105**, 037002 (2010).
- [5] J. O. Sofo, A. S. Chaudhari, G. D. Barber, Phys. Rev. B **75**, 153401 (2007).
- [6] D. C. Elias *et al.*, Science **323**, 610 (2009).
- [7] P. Giannozzi *et al.*, J. Phys.: Condens. Matter **21**, 395502 (2009).
- [8] P. Giannozzi *et al.*, J. Phys.: Condens. Matter **29**, 465901 (2017).
- [9] S. Poncé, E. R. Margine, C. Verdi, F. Giustino, Comput. Phys. Commun. **209**, 116 (2016).
- [10] D. K. Efetov, P. Kim, Phys. Rev. Lett. **105**, 256805 (2010).
- [11] V. M. Loktev, V. Turkowski, J. Low Temp. Phys., doi:10.1007/s10909-011-0376-7 (2011).