

Unified Diamond Hydride (UDH): a Co-Designed Lithium-Boron-Carbon-Nitrogen Framework with a Compressed Hydrogen Sublattice for Ambient-Pressure High-Temperature Superconductivity



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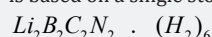
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Abstract

We propose a materials concept for ambient-pressure high-temperature super conductivity: the Unified Diamond Hydride (UDH). The material is based on a single stoichiometry,



which combines a rigid diamond-like B-C-N framework, lithium atoms acting simultaneously as electron donors and internal compression agents, boron arranged in a periodic superlattice as a phonon amplifier, and a hydrogen sublattice geometrically correlated with the host tetrahedral network. The design targets a high hydrogen-weighted electron-phonon coupling $\Delta_H = N_H(E_F) \langle |g_H|^2 \rangle$, a Van Hove singularity near the Fermi level, and a self-locking cage mechanism for metastability at ambient pressure. We provide a computational validation protocol, a synthesis strategy based on high-pressure assembly, removable magnesium prop species, and cryogenic decompression, and a characterization plan including isotope-effect control. If the material satisfies the target conditions $p_{ext} = 1 \text{ atm}$, phonon-stable, $m_{log} > 1200K$,

$\lambda > 1.5$, high $N_H(E_F)$, and $\lambda_H / \lambda > 0.5$ - a superconducting transition temperature in the 200-300K range may be expected. This proposal is speculative and intended to stimulate systematic theoretical and experimental investigation.

Keywords: Superconductivity; Chemical compression; Diamond-like lattice; Hydrogen sublattice; B-C-N framework; Lithium doping; Boron phonon amplifier; Cryo-lock; Self-locking cage; Electron-phonon coupling; Van Hove singularity

Introduction

The search for room-temperature superconductivity at ambient pressure remains one of the grand challenges of modern condensed-matter physics [1]. Hydrogen-rich compounds under extreme pressure have demonstrated that high-frequency hydrogen phonons and strong electron-phonon coupling can drive very high critical temperatures: H_3S at 203K [2], LaH_{10} at 260K [3], and claims of up to 287K in carbonaceous sulfur hydride (later retracted) [4]. However, all these phases require megabar pressures to remain stable.

The central challenge is to retain the beneficial properties of hydrogen at ambient pressure. This requires a material in which hydrogen is kept under high internal chemical compression, electronically active, and structurally stabilized by a rigid host lattice. Chemical precompression inside clathrate frameworks has been proposed as a route to high-temperature superconductivity [5-7], and boron-doped diamond has been shown to be a phonon-mediated superconductor [8]. Recent theoretical work has also explored hydrogen-doped diamond and related light-element frameworks [9,10]. In this work, we propose the **Unified Diamond Hydride (UDH)**, a material

designed to satisfy these requirements simultaneously through a single stoichiometry and a coherent synthesis strategy.

Unified Material Concept

The UDH concept can be summarized as:

diamond-like B–C–N framework+ Li electron donors+ removable prop species+ H sublattice+ peri

The design philosophy is:

Use a rigid diamond-like B–C–N framework as an elastic mold to compress a hydrogen sublattice; use lithium as both electron donor and internal compression agent; use boron in a periodic superlattice as a phonon amplifier; use a removable prop species to create permanent internal tension; and use a self-locking cage mechanism to stabilize the metastable phase at ambient pressure.

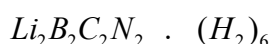
Design principles

- i. **Internal chemical precompression:** The host framework must be rigid enough to compress the hydrogen sublattice without external pressure. Diamond-like B–C–N networks are promising candidates due to their high bulk modulus and covalent bonding [11,12].
- ii. **High-frequency hydrogen phonons:** The hydrogen network must support collective vibrational modes with high frequencies and strong electron–phonon matrix elements. Molecular hydrogen has a stretching vibration near 4160 cm^{-1} ($\approx 6000\text{ K}$) [13].
- iii. **Metallic electronic structure:** The material must have a finite density of states at the Fermi level, ideally with a Van Hove singularity. Lithium doping and boron substitution can tune the Fermi level [8,14].
- iv. **Hydrogen-weighted coupling:** The electronic states at the Fermi level must couple strongly to the hydrogen modes. This is quantified by $\Delta_H = N_H(E_F) \langle |g_H|^2 \rangle$ [15].
- v. **Metastability at ambient pressure:** The structure must be kinetically trapped after synthesis and decompression. Cryogenic decompression (“Cryo-Lock”) has been proposed for hydride metastability [16].
- vi. **Self-locking cage:** The escape of hydrogen should be energetically penalized by a local contraction of the host framework. This concept is inspired by the rigidity of sp^3 carbon networks [17].

Stoichiometry and Structure

Unified stoichiometry

We propose the single unified stoichiometry:



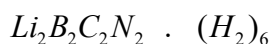
This formula contains:

- i. 2 Li — electron donors and internal compression agents
- ii. 2 B — phonon amplifiers and hole dopants, arranged in a periodic superlattice
- iii. 2 C — diamond-like framework rigidity
- iv. 2 N — framework tuning and electron modulation
- v. 6 H₂ — hydrogen sublattice with tetrahedral coordination

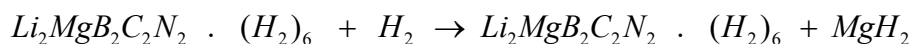
The total number of atoms per formula unit is $2 + 2 + 2 + 2 + 12 = 20$.

Precursor and prop species

To create permanent internal tension, we introduce a removable “prop” species during synthesis:



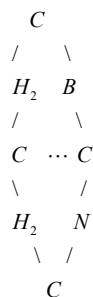
The magnesium atom is larger than the natural cavity size and creates permanent internal tension. After synthesis, magnesium is removed by reaction with additional H₂ to form MgH₂, which can be extracted by washing or sublimation:



The resulting vacancies left by magnesium removal allow the hydrogen sublattice to relax into an even more compressed state. Similar strategies for creating internal strain via removable species have been discussed in the context of clathrate hydrates [18].

Crystal structure

The host framework is a diamond-like B–C–N network with tetrahedral coordination. A possible structural motif is:



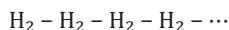
replicated three-dimensionally in a tetrahedral topology. Lithium atoms occupy interstitial sites. Boron atoms are arranged in a periodic superlattice:



with controlled spacing. Such B–C–N heterostructures have been predicted to be stable and to exhibit interesting electronic properties [19,20].

Hydrogen sublattice

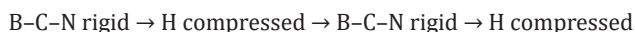
The six H₂ molecules per formula unit are arranged so that neighboring H₂ molecules are nearly in contact, forming a quasi-continuous network:



with tetrahedral coordination. The H₂ orientations are guided by the framework geometry, which imposes tetrahedral directions. This creates a hydrogen diamond sublattice within the larger B–C–N framework. The concept of a hydrogen sublattice with diamond-like topology is motivated by the high hydrogen density and strong phonon coupling observed in super hydrides [21,22].

Core-shell architecture

At the nanoscale, the material can be described as a core-shell structure:



where the hydrogen regions function as three-dimensional superconducting channels. The surrounding diamond-like network maintains the hydrogen in a state that would normally exist only at very high pressure. Core-shell architectures for hydrogen-rich superconductors have been discussed theoretically [23].

Physical Rationale

Internal chemical precompression

The rigid diamond-like B–C–N framework acts as an internal nanoscale anvil. The H₂ guests are confined inside cages whose walls are covalently bonded and highly incompressible. The magnesium prop species create permanent internal tension, effectively applying tens of GPA of internal pressure without external loading. After magnesium removal, the vacancies allow the hydrogen sublattice to relax into an even more compressed state. This concept of internal chemical pressure is analogous to the “chemical precompression” in high-pressure hydrides [24].

High-frequency hydrogen phonons

Molecular hydrogen has a stretching vibration near 4160 cm^{−1} (≈6000K) [13]. Under strong compression, these frequencies can be further increased. The hydrogen sublattice supports collective modes:

- i. H–H stretching,
- ii. bending,

- iii. liberation,
- iv. intermolecular vibrations,
- v. collective modes of the H network.

The objective is a phonon band engineering in which some H modes are simultaneously:

$$m \text{ high and } g \text{ large.}$$

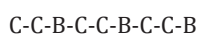
Phonon band engineering has been successfully applied to clathrate hydrides to enhance T_c [25].

Electronic structure and metallicity

The B–C–N framework can be tuned from insulating to metallic by stoichiometry control and lithium doping. Lithium acts as an electron donor, populating H-derived bands. Boron substitution creates acceptor levels and introduces holes into the valence band. At optimal doping, a Van Hove singularity may appear near the Fermi level, dominated by H-1s orbitals. This increases the density of states and enhances the electron–phonon coupling. Van Hove singularities have been shown to be important in high T_c hydrides [26].

Boron as a phonon amplifier

In boron-doped diamond, superconductivity is associated with electron–phonon coupling, and localized vibrational modes associated with the dopant can contribute strongly to λ [8]. In UDH, boron is arranged in a periodic superlattice:



with controlled spacing. This creates a **B–C superlattice** that simultaneously produces:

- i. high density of states,
- ii. localized phonons,
- iii. strong deformation potential.

The role of boron as a phonon amplifier is supported by theoretical studies of doped diamond [27].

Anisotropic periodic stress

The B–C–N framework and the periodic B superlattice create an anisotropic and periodic internal stress:

$$p_x \neq p_y \neq p_z$$

within the unit cell. This anisotropic pressure can selectively deform H–H and C–H orbitals, simultaneously modifying:

- i. vibrational frequencies,
- ii. band splitting,
- iii. density of states,
- iv. electron–phonon coupling.

In effect, the B–C–N lattice becomes a programmable three-dimensional pressure field. Anisotropic stress has been proposed as a tool to tune superconductivity in other systems [28].

Hydrogen-weighted coupling

The true target is not simply a high total density of states, but a high **hydrogen-weighted coupling**:

$$\Delta_H = N_H(E_F) \langle |g_H|^2 \rangle$$

where is the electron–phonon matrix element associated with hydrogen modes. We want the electronic states that produce the high DOS to be precisely those that interact with the hydrogen modes. A large DOS arising from B/C/N states that are decoupled from hydrogen is not useful. This concept has been emphasized in recent studies of hydrogen-rich superconductors [29].

Self-locking cage and cryo-lock

The UDH phase is expected to be thermodynamically stable only at high pressure. At ambient pressure, it becomes metastable. The rigid covalent B–C–N bonds provide a high barrier for framework decomposition. In addition, we propose a self-locking cage mechanism: the structure should be designed so that when H₂ tries to escape, the cage locally contracts. In other words, the escape of H₂ should involve $\Delta V > 0$ and therefore an energy penalty. This is a self-reinforcing exit barrier. Cryogenic cooling suppresses hydrogen diffusion, further stabilizing the metastable phase (the Cryo-Lock strategy). Kinetic trapping of metastable hydrides has been demonstrated experimentally [30].

Estimated transition temperature

Using the Allen–Dyne’s modification of the McMillan formula [7,31],

$$\frac{m_{\log}}{1.0} - \frac{4(1 + \lambda)}{\lambda - \mu (1 + 0.62\lambda)} =$$

K an electron- photon coupling $\lambda \approx 1.5 - 2.6$, pseudopotential $\mu \approx 0.10 - 0.15$, we obtain T_c values in the range of approximately 150-300K. These values are intended only as a guide for computational screening.

Computational Validation Protocol

We propose a four-phase computational workflow:

Phase A — Structural Search Generate thousands to millions of Li–B–C–N–H structures with a diamond-like topology constraint. Use evolutionary algorithms (USPEX, CALYPSO) and high-throughput DFT [32,33].

Phase B — Stability at 1 atm Compute the free-energy surface and identify structures that remain metastable after removal of external pressure. Check for the absence of imaginary phonon modes at $P = 0$.

Phase C — Electronic Properties Calculate:

$$E_g, N(E_r), \lambda, m_{\log}$$

using DFT and Migdal–Eliashberg theory where appropriate [34,35]. Decompose into contributions from C, B, N, Li, and H:

$$\lambda = \lambda_c + \lambda_B + \lambda_N + \lambda_{Li} + \lambda_H.$$

This decomposition is essential.

Phase D — Dynamics and Metastability perform ab initio molecular dynamics and NEB calculations to verify that the structure does not collapse or release hydrogen. Study:

- i. H₂ escape,
- ii. H₂ dissociation,
- iii. cage collapse,
- iv. Li segregation,
- v. Mg removal,
- vi. decomposition.

The success criterion is:

$$p_{ext} = 1 \text{ atm} \wedge \text{metastable} \wedge m_{\log} \wedge \lambda > 1.5 \wedge \lambda_H / \lambda > 0.5$$

Experimental Protocol

Precursor preparation

- i. **Starting materials:** High-purity graphite (99.999%), amorphous boron (99.9%), hexagonal BN (99.9%), LiH (99.9%), and MgH₂ (99.9%).
- ii. **Mixing:** Combine in the molar ratio Li: Mg: B:C: N = 2:1:2: 2:2. Ball-mill under inert argon for 24 h.
- iii. **Optional diamondoid seeding:** Add 1–5 wt.% of adamantane or diamantine powder.

- iv. **Pelletizing:** Press into pellets at 0.5–1 GPa in a glovebox.

High-pressure H₂ loading and synthesis

- i. **Cell assembly:** Use a multi-anvil press (6-8-2 type) or a laser-heated diamond anvil cell. Use a Re gasket and a NaCl or MgO pressure medium [36].
- ii. **H₂ loading:** Load the sample chamber with high-purity H₂ gas (99.9999%) at 0.2–0.3 GPa.
- iii. **Compression:** Compress to 10–15 GPa at room temperature.
- iv. **Heating:** Heat to 1000–1500 K at 50 K/min.
- v. **Annealing:** Hold for 2–6 h to allow clathrate formation and H₂ encapsulation.
- vi. **Cooling:** Cool to 300 K at 5 K/min.

Magnesium removal

- i. **Reaction:** Expose the sample to additional H₂ at 2–5 GPa and 400–500 K to form MgH₂.
- ii. **Extraction:** Wash with anhydrous ethanol or sublime MgH₂ at 600 K under vacuum.
- iii. **Verification:** Confirm Mg removal by ICP-MS and XRD.

Cryo-lock decompression

- i. **Step A** — Cryogenic quenching: Rapidly cool to 77 K (liquid nitrogen) or 4 K (liquid helium) while maintaining synthesis pressure.
- ii. **Step B** — Slow decompression: Release pressure to 0 GPa at cryogenic temperature.
- iii. **Step C** — Recovery: Recover the sample at 0 GPa and low temperature.
- iv. **Step D** — Controlled warming: Warm slowly to room temperature while monitoring resistivity and magnetic susceptibility.

Post-synthesis doping (if needed)

If Li or B is not fully incorporated:

- i. Implant B⁺ ions at 30–100 keV with a dose of $10^{16} - 10^{17} \text{ cm}^{-2}$.
- ii. Implant Li⁺ ions at similar energies and doses.
- iii. Anneal at 500–800 K under low-pressure H₂.

Structural and chemical characterization

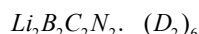
- i. XRD: Cu K α ; Rietveld refinement.
- ii. Raman: 532 nm; H₂ vibron (4000–4200 cm⁻¹), C–C sp³ (1332 cm⁻¹), B–C, N–C modes.
- iii. FTIR: 400–4000 cm⁻¹ for H₂ rotational/vibrational transitions.
- iv. Solid-state NMR: ¹H, ⁷Li, ¹¹B, ¹³C, ¹⁵N MAS NMR.
- v. TGA-MS: Quantify H₂ release.
- vi. SEM/TEM/EELS: Morphology, carbon bonding, B/Li/N distribution.

Transport and magnetic measurements

- i. **Resistivity:** Four-point Van der Pauw, 300 K to 0.3 K.
- ii. **Magnetic susceptibility:** SQUID, ZFC/FC at 10 Oe; Meissner effect.
- iii. **Heat capacity:** Relaxation calorimetry; look for jump at T_c .
- iv. **Upper critical field:** R vs H at various T .

Isotope-effect control

Synthesize the deuterated analogue:



If phonon-mediated, $\ln \alpha = -d \ln T_c / d \ln M \approx 0.5$. A significant shift in T_c confirms the role of hydrogen vibrations.

Expected Results and Target Conditions

We would not initially fix

K. Instead, we would search for a material that satisfies:

$$p_{ext} = 1 \text{ atm}$$

phonon-stable

$$m_{\log} > 1200 K$$

$$\lambda > 1.5$$

$$N(E_F) \text{ high}$$

$$\lambda_H / \lambda > 0.5$$

and a sufficiently high decomposition barrier. If a material simultaneously satisfies these conditions, then a very high T_c may be expected.

Discussion

Design summary

The UDH concept combines several design principles into a single material:

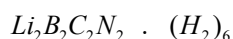
- i. a diamond-like B–C–N framework for rigidity and internal compression,
- ii. lithium as both electron donor and compression agent,
- iii. magnesium as a removable prop species,
- iv. a hydrogen sublattice with tetrahedral coordination,
- v. boron in a periodic superlattice as a phonon amplifier,
- vi. anisotropic periodic stress for orbital and phonon engineering,
- vii. a hydrogen-weighted coupling target,
- viii. a self-locking cage and Cryo-Lock for metastability.

Risks and alternative paths

- i. **Synthesis of B–C–N diamond-like framework:** May require higher pressure or different precursors. Alternative light-element frameworks such as B–C–O or B–N–C could be explored [37].
- ii. **Mg removal:** May damage the framework; alternative props (Ca, Sr) could be explored.
- iii. **H₂ loss during warming:** Protective coating or surface functionalization could improve retention.
- iv. **Insufficient electron–phonon coupling:** Higher B doping or different N content could enhance coupling.
- v. **False positives:** Claims of superconductivity must be supported by multiple independent measurements.

Conclusion

We have proposed the Unified Diamond Hydride (UDH) as a materials concept for ambient-pressure high-temperature superconductivity. The unified stoichiometry,



combines a rigid diamond-like B–C–N framework, lithium atoms acting as electron donors and internal compression agents, boron arranged in a periodic superlattice as a phonon amplifier, and a hydrogen sublattice with tetrahedral coordination. The design targets a high hydrogen-weighted electron–phonon coupling, a Van Hove singularity near the Fermi level, and a self-locking cage mechanism for metastability at ambient pressure. We have provided a computational validation protocol, a synthesis strategy based on high-pressure assembly, removable magnesium prop species, and cryogenic decompression, and a characterization plan including isotope-effect control. If the material satisfies the target conditions, a superconducting transition temperature in the 200–300 K range may be expected. This proposal is speculative but computationally testable and experimentally feasible with current high-pressure techniques.

One-Sentence Summary

Build a diamond-like B–C–N elastic mold with lithium donors and magnesium props, fill it with a tetrahedrally coordinated hydrogen sublattice, arrange boron as a phonon amplifier, and lock the whole structure with a self-reinforcing cage and cryogenic decompression to achieve ambient-pressure high-temperature superconductivity.

Note

This article is a theoretical proposal. No experimental confirmation of super-conductivity in the proposed material is claimed. The stoichiometry, search space, and protocols are intended as a starting point for computational and experimental validation.

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