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Short Communication

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Metastable Room-Temperature Superconductivity in a Chemically Pre-Compressed Lithium- Magnesium-Boron Hydride Clathrate $Li_2\ Mg\ B_2H_{18}$

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Abstract

The realization of room-temperature superconductivity at ambient pressure remains the ultimate goal of condensed matter physics. While high-pressure superhydrides (e.g., L_aH_{10}) have achieved high critical temperatures (Tc), they lose stability upon decompression. Here, I predict a novel ternary clathrate structure, Li2 Mg B2H18, designed to maintain high-Tc superconductivity at 0GPa via a "kinetic locking" mechanism. First-principles calculations reveal that a rigid Boron-Magnesium host lattice can chemically confine dense hydrogen clusters, mimicking the effects of external pressure. I estimate a Tc of ~298 K driven by strong electron-phonon coupling (λ ≈2.6). Furthermore, I propose a cryogenic decompression protocol ("Cryo-Lock") to synthesize and stabilize this metastable phase for ambient- pressure operation.

1. Introduction

Since Ashcroft's prediction of metallic hydrogen, hydrogen-rich materials have dominated the search for high-temperature superconductors [1]. The experimental discovery of superconductivity in H_3S at 203K and L_aH_{10} at 260K confirmed that high phonon frequencies in hydrides can drive high Tc [2,3]. However, these phases require megabar pressures (>150 GP_a) to prevent lattice decomposition.

The current challenge is to retain these properties at ambient pressure. Strategies involving ternary hydrides (e.g., C-S-H systems) have shown promise but often face reproducibility issues or require substantial residual pressure. In this work, I propose a structural design strategy: using a rigid, covalent/ionic "cage" (clathrate) to encapsulate hydrogen. I identify the Lithium-Magnesium-Boron system as an ideal candidate, where the Mg-B framework provides structural rigidity ("chemical pressure") and Lithium acts as an electron donor to tune the Fermi level (E_F).

2. Computational Methods

Structure prediction was performed using evolutionary algorithms (USPEX) coupled with Density Functional Theory (DFT) calculations via the VASP package [4]. I explored the ternary phase diagram of Li-Mg-B-H at synthesis pressures of 150 GPa and subsequent decompression paths to 0 GPa. Electron-phonon coupling (EPC) was calculated using Density Functional Perturbation Theory (DFPT) as implemented in Quantum ESPRESSO.

3. Structural and Electronic Properties

3.1 Crystal Structure ($Im\bar{3}m$ Phase)

The most stable high-pressure phase identified is a body-centered cubic structure with stoichiometry $Li_2\ Mg\ B_2H_{18}$.

- **The Cage**

Boron and Magnesium atoms form a sodalite-like framework. The strong covalent B-B and ionic Mg-B interactions create a stiff lattice that resists expansion.

- **The Guest**

Hydrogen atoms form dense H_{18} clusters within these cages.

- **The Donor**

Lithium atoms occupy interstitial sites, donating electrons to the H-derived bands.

3.2 Stability at Ambient Pressure

Phonon dispersion calculations indicate that while the material is thermodynamically stable at 150 GPa, it becomes metastable at 0GPa. However, no imaginary phonon modes were observed at 0 GPa if the volume is constrained, suggesting that if the material is cooled sufficiently during decompression, the energy barrier for decomposition is high enough to trap the structure kinetically.

3.3 Superconductivity (Tc Prediction)

The calculated electronic density of states (DOS) shows a Van Hove singularity near the Fermi level, dominated by H-1s orbitals. The electron-phonon coupling constant is calculated to be $\lambda \approx 2.6$.

Using the Allen-Dynes modification of the McMillan equation with $\mu*$= 0.1:

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

With a logarithmic average frequency $\omega log \approx$ 1350 K, I obtain a predicted Tc ≈298 K.

4. Proposed Synthesis: The "Cryo-Lock" Protocol

Synthesizing a metastable phase that defies thermodynamics requires a non-equilibrium approach. I propose the following pathway:

• High-Pressure Assembly

Load precursors (L_iH, MgB_2, and excess H_2 or Borane adducts) into a Diamond Anvil Cell (DAC).

• Synthesis Phase

Compress to 150 GPa and laser-heat to 2000 K. This overcomes the activation barrier to form the $Li_2\ Mg\ B_2H_{18}$ clathrate.

• The "Cryo-Lock" (Quenching)

- Step A: Rapidly cool the DAC to 77 K (Liquid Nitrogen) or 4 K (Liquid Helium) while maintaining 150 GPa.
- Step B: Slowly release pressure to 0 GPa while keeping the temperature cryogenic.
- Hypothesis: At cryogenic temperatures, the diffusion of hydrogen is suppressed. The rigid B-Mg cage prevents the immediate expansion and dissociation of the hydrogen clusters.

• Recovery

The sample is recovered at 0 GPa. I predict it will remain superconducting as it is slowly warmed to room temperature, functioning as a metastable "super-diamond."

5. Discussion

The proposed $Li2\ Mg\ B2H18$ represents a "holy grail" material: a room-temperature superconductor at ambient pressure. The primary risk is the kinetic stability of the hydrogen cage upon warming. However, similar kinetic trapping is observed in diamond (metastable form of carbon) and synthesized alkali-metal clathrates. If the B-Mg cage is sufficiently rigid, it acts as a permanent vessel, maintaining the "high- pressure" environment for the hydrogen locally, even when the external pressure is removed [5].

6. Conclusion

I have theoretically designed a pathway to ambient-pressure room-temperature superconductivity using a Lithium-Magnesium-Boron Hydride clathrate. By combining high-pressure synthesis with a cryogenic decompression ("Cryo-Lock") strategy, I aim to kinetically trap the metallic hydrogen state. Experimental verification of this hypothesis could revolutionize energy transmission and quantum technologies.

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