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Theoretical Prediction and Synthesis Pathway for a Metastable Yttrium-Carbon-Hydride (Y–C–H) Superconductor at High Pressures

Giustino Travaglini

Independent Researcher, Italy

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Abstract

The pursuit of room-temperature superconductivity has recently been dominated by the high-pressure phases of hydrogen-rich materials, such as H_3S and LaH_{10}. While these binary hydrides exhibit remarkably high critical temperatures (Tc), their stabilization often requires pressures exceeding 150 GPa, limiting their practical scope. In this work, I propose a novel ternary system, Yttrium-Carbon-Hydride (Y–C–H), as a promising candidate for high-Tc superconductivity at reduced pressures. Based on Density Functional Theory (DFT) and evolutionary algorithm predictions, I identify a clathrate-like, face-centered cubic phase with an approximate composition of $YC_{0.2}$. H_{10}that is dynamically stable above 50 GPa. My calculations indicate a strong electron-phonon coupling mechanism, primarily driven by the high- frequency hydrogen vibrations, leading to a predicted Tc of up to 220 K at 100 GPa. I further detail a comprehensive experimental synthesis protocol using a diamond anvil cell (DAC) with in-situ laser heating and characterization, providing a roadmap for the empirical validation of this theoretically proposed material.

Corresponding author: Giustino Travaglini, Independent Researcher, Italy.

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Introduction

Superconductivity in hydrogen-dominated compounds under high pressure represents a paradigm shift in condensed matter physics. The chemical pre-compression offered by elements like S or La in H_3S and LaH_{10}, respectively, facilitates the metallization of hydrogen at accessible pressures, resulting in phonon- mediated superconductivity with Tc values approaching ambient conditions [1, 2]. However, the extreme pressures required for these phases (>150 GPa) present a significant experimental bottleneck. A promising strategy to mitigate this is the introduction of a third element to act as a chemical pressure agent and electronic dopant, potentially stabilizing high-Tc phases at lower physical pressures. This approach has been explored in systems like C–S–H [3] and Lu–N–H [4], albeit amidst ongoing debate regarding their reproducibility.

In this paper, I turn my attention to the Y–H system, known for high-Tc phases like YH_6 and YH_9 [5], and propose the incorporation of carbon as a ternary constituent. Carbon, with its small atomic radius and propensity for strong covalent bonding, is hypothesized to introduce beneficial chemical strain and modify the electronic density of states at the Fermi level. I present a first-principles study predicting the stability and superconducting properties of Y–C–H and propose a detailed protocol for its synthesis.

Computational Methods & Theoretical Prediction

My initial investigation relied on ab-initio calculations within the framework of Density Functional Theory (DFT) as implemented in the VASP code [6]. The electron-ion interaction was described by the projector augmented-wave (PAW) method, and the generalized gradient approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) form was used for the exchange-correlation functional.

To explore the configurational space, I employed the USPEX evolutionary algorithm [7] for crystal structure prediction at pressures of 50, 100, and 150 GPa. The search focused on stoichiometries around YC_xH_{10} ($x = 0.1–0.5$). The most promising candidate identified was a face-centered cubic (FCC)

structure (space group *Fm-3m*) with an approximate composition of $YC_{0.2}H_{10}$, where carbon atoms occupy specific interstitial sites within a Y–H lattice.

The phonon dispersion spectra confirmed the dynamical stability of this phase above 50 GPa. The electron-phonon coupling constant (λ) was calculated to be 2.1, and the logarithmic average frequency (ω_log) was 1250 K. Using the McMillan-Allen-Dynes formula, I estimated a Tc of 220 K at 100 GPa.

Proposed Experimental Synthesis Protocol

The synthesis of this metastable Y–C–H phase requires a combination of high pressure and controlled thermal activation.

Precursor Preparation

High-purity Yttrium powder (99.99%), Fullerene C_{60}(99.9%), and Magnesium Hydride (MgH_2, 99.9%) will be used as precursors. They will be mixed in a molar ratio of Y : C_{60}: MgH_2= 1 : 0.033 : 5 inside an argon-filled glovebox (O_2& H_2O < 0.1 ppm). This ratio targets the $YC_{0.2}H_{10}$composition, with MgH_2acting as a solid-state hydrogen source.

High-Pressure Synthesis in Diamond Anvil Cell (DAC)

The mixture will be loaded into a diamond anvil cell (DAC) equipped with 300-400 μm culet diamonds. A rhenium gasket will be used, with a ruby sphere for pressure calibration via the fluorescence method.

Step 1 (Compression): The sample will be compressed to a target pressure of 2 GPa to ensure initial compactness.

Step 2 (Laser Heating): The sample will be subjected to laser heating at a wavelength of 1070 nm. A multi-step thermal treatment is proposed:

Stage A (Decomposition): 1200 K for 2 minutes to decompose MgH_2($MgH_2 \rightarrow Mg + H_2$).

Stage B (Reaction): Increase pressure to 50-100 GPa, followed by rapid laser heating to 1800-2000 K for 30-60 seconds. This provides the energy for C_{60}cage collapse and atomic diffusion to form the ternary phase.

Stage C (Annealing): Slow cooling to 1000 K to anneal the sample and promote crystalline order.

In-Situ Characterization and Superconductivity Testing The success of the synthesis will be monitored in real-time:

In-Situ X-Ray Diffraction (XRD): To confirm the formation of the predicted FCC phase and rule out the presence of binary byproducts (e.g., YH_6, YC_2, or graphite).

In-Situ Raman Spectroscopy: To track the disappearance of C_{60} and MgH_2 peaks and the emergence of Y–H and C–H vibrational modes.

Following synthesis, the superconducting properties will be characterized:

Resistivity Measurements: A four-point probe method will be used to measure the electrical resistance as a function of temperature. A sharp drop to zero resistance is the primary indicator of superconductivity.

Meissner Effect Measurement: The magnetic susceptibility will be measured to observe the diamagnetic response below Tc, providing definitive proof of the superconducting state.

Discussion and Outlook

The proposed Y–C–H system represents a rational extension of the "chemical pressure" paradigm in hydride superconductors. The theoretical prediction of a Tc of 220 K at 100 GPa, while not at ambient temperature, would place this material among the highest-Tc superconductors known, with the potential advantage of stability at significantly lower pressures than LaH_{10}.

Potential challenges include the separation of elemental phases (e.g., formation of thermodynamically favored YC_2) and the metastability of the phase upon pressure release. However, even a successful synthesis at high pressure would validate a new material class and provide invaluable insights for future explorations, such as doping with other light elements (e.g., B, N) or exploring different metal hosts (e.g., Sc, Lu).

Conclusion

I have theoretically proposed a novel ternary superconductor, $YC_{0.2}H_{10}$, and provided a detailed, experimentally feasible roadmap for its synthesis. My DFT calculations predict a high Tc of 220 K at 100 GPa. This work not only identifies a specific promising compound but also establishes a general

strategy for designing high-Tc hydrides at reduced pressures by employing carbon as a chemical modifier. Experimental efforts to realize this material are currently being initiated.

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