

Underlying mechanism for high-temperature superconductivity in ternary hydride AB_2H_{24} Bowen Jiang^{1,2}, Xin Zhong^{1,*} and Hanyu Liu^{1,2,3,†}¹Key Laboratory of Material Simulation Methods and Software of Ministry of Education, College of Physics, Jilin University, Changchun 130012, China²State Key Laboratory of Superhard Materials, College of Physics, Jilin University, Changchun 130012, China³International Center of Future Science, Jilin University, Changchun 130012, China

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Recent studies have highlighted the potential for achieving room-temperature superconductivity in the clathrate hydride prototype AB_2H_{24} with the $P6/mmm$ space group symmetry. To investigate the underlying superconducting mechanism for this class of frameworks, we performed comprehensive first-principles calculations by systematically substituting metal elements from groups I to IV of the periodic table. The results identify 21 dynamically stable compounds at 300 GPa, exhibiting an extraordinary variation in superconducting critical temperatures (T_c), ranging from 276 K in $AcSc_2H_{24}$ to 2 K in $ThCe_2H_{24}$. Through detailed structural analysis, we proposed two key model parameters, S_{couple} and coupling strength (CS), to elucidate the strong correlation with superconducting properties (showing correlation coefficients of 0.87 and 0.93 with respect to T_c). These model parameters are further demonstrated to be extendable for other clathrate-type hydrides, such as $Li_2MH_{16/17}$ and binary superhydrides MH_6 , MH_9 and MH_{10} . The proposed CS shows strong predictive capability, achieving an overall correlation coefficient of 0.85 across different clathrate hydride systems. These findings provide insights into the fundamental mechanisms governing the superconducting properties of clathrate hydrides, offering useful guidance for future superconductor design.

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I. INTRODUCTION

The pursuit of high-temperature superconductors has been a century-long endeavor in condensed matter physics. Recent discoveries in hydride superconductors with critical temperatures (T_c) above 200 K underscore the possibility of achieving room-temperature superconductivity under high pressures [1,2]. Since the first-ever clathrate superhydride CaH_6 was predicted to have high- T_c values of 220–235 K at 150 GPa [3–5], several binary clathrate superhydrides have been predicted through advanced crystal structure prediction methods [6,7] and confirmed experimentally, such as LaH_{10} , YH_6 , and YH_9 [3,4,8–13]. These discoveries have sparked great interest in exploring hydrides with more complex and diverse compositions [1,14–17]. For instance, by introducing extra lithium into the Mg-H system, the T_c of Li_2MgH_{16} can reach 473 K at 250 GPa [18]. Similarly, Li_2ScH_{16} (281 K at 230 GPa), Li_2YH_{16} (285 K at 170 GPa), and Li_2CaH_{16} (330 K at 350 GPa) [19,20], which share the same structural framework as Li_2MgH_{16} , also exhibit T_c 's exceeding room temperature under high pressures. More recently, $LaSc_2H_{24}$

and ThY_2H_{24} have been predicted to be thermodynamically stable below 200 GPa, with high T_c 's surpassing room temperature [21,22]. These findings highlight the potential of ternary clathrate hydrides as promising candidates in the search for high- T_c superconductors and emphasize the crucial role of structural and compositional tuning in optimizing superconducting properties.

The clathrate superhydrides are characterized by nested cage units formed by hydrogen atoms, with an H-H distance of approximately 1.0 Å, and metal atoms occupying the center of the cage units [1,23]. The metal atoms play a role in donating electrons to hydrogen atoms and fine-tuning the distribution of hydrogen bond lengths. Previous studies have demonstrated that substituting different metal atoms within the same hydrogen framework can lead to significant variations in both superconducting properties and stability. These effects are well exemplified by a series of binary clathrate hydrides, such as MH_6 , MH_9 , and MH_{10} superconductors [10,11,24–27]. Generally, the T_c values exhibit a positive correlation with the density of states at the Fermi level contributed by hydrogen ($PDOS_H$; projected density of states on hydrogen), as well as the lowest pressure at which the structure remains dynamically stable. These variations are primarily driven by the choice of metal elements. Therefore, a deeper understanding of how these metal atoms influence the properties of clathrate hydride superconductors is essential for the design of high- T_c superconductors.

In recent studies, the high-temperature superconductors $LaSc_2H_{24}$ and ThY_2H_{24} were predicted to exhibit theoretical T_c 's of 316 K at 167 GPa and 303 K at 150 GPa [21,22],

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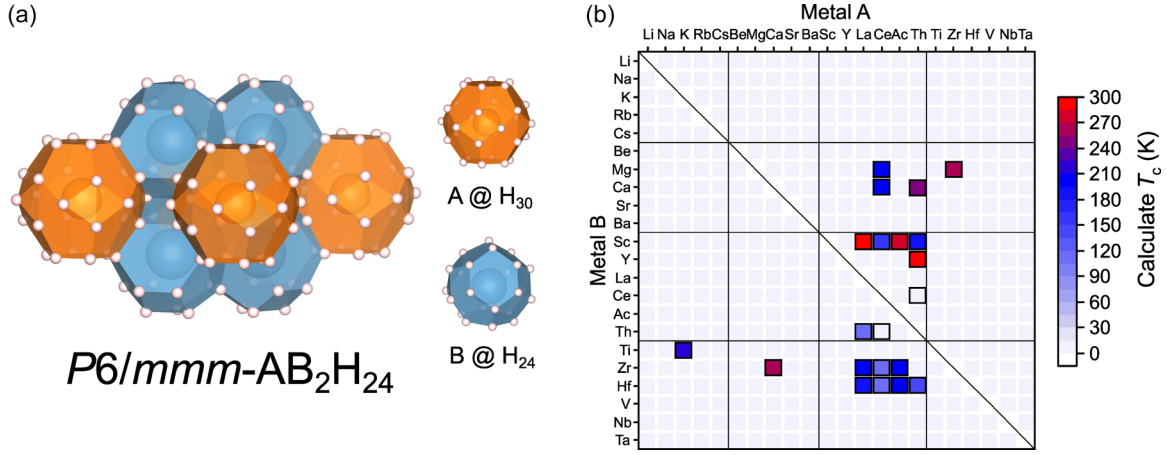


FIG. 1. (a) The framework of $P6/mmm-AB_2H_{24}$, which consists of two types of cages, showing two types of hydrogen cages highlighted in orange and blue. The larger metal A is located in the orange cage and the smaller metal B is located in the blue cage. (b) Predicted superconducting properties of different metal element combinations. Combinations that are dynamically stable are marked with black-bordered squares.

respectively. Motivated by these encouraging findings, we selected this structural framework as the basis for our investigation. We systematically substituted metal elements from Groups I–IV of the periodic table. Using first-principles calculations, we examined more than 462 ternary compounds at 300 GPa and identified 21 dynamically stable structures with T_c values ranging from 2 to 300 K. Based on these computational results, we further analyzed their electronic and structural properties. We introduced two empirical parameters to describe the superconducting behavior of clathrate hydrides. The first, S_{couple} , is defined as the product of the electron localization function (ELF) and the corresponding H–H bond length:

$$S_{\text{couple}} = \text{ELF} \times \text{bonds}.$$

The second parameter, CS (coupling strength), linearly combines S_{couple} with the PDOS_H:

$$\text{CS} = A \times \text{PDOS}_H + B \times S_{\text{couple}}.$$

These descriptors incorporate the values of PDOS_H, the ELF values between hydrogen bonds, and the values of H–H bond length, providing a quantitative assessment of the correlation between structural features and T_c values. A linear fit yields a correlation coefficient of 0.93 between CS and T_c in AB_2H_{24} -type clathrate superhydrides, highlighting the predictive capability of the model. Furthermore, our in-depth analysis demonstrated that this parameter model is also applicable to other clathrate-type systems, including ternary frameworks such as $\text{Li}_2\text{MH}_{16/17}$ and binary superhydrides such as MH_6 , MH_9 , and MH_{10} . Across all the systems, the model maintains a robust overall correlation coefficient of 0.85. These results suggest that our model effectively captures the intrinsic superconducting mechanisms of clathrate superhydrides, offering valuable insights into the nature of superconductivity and guiding the future design of high- T_c materials.

II. COMPUTATIONAL DETAILS

Based on the prototype of $P6/mmm\text{-LaSc}_2\text{H}_{24}$, we initially selected metal elements from Groups I–IV of the periodic table, including La, Ce, Ac, and Th, to permutationally occupy the sites of La and Sc atoms (see Fig. 1). A total of 462 structures were generated and subsequently optimized at 300 GPa using the VASP (Vienna *Ab initio* Simulation Package) [28]. The dynamic stabilities were further assessed using the finite displacement method and postprocessed with the vaspkit code [29]. The exchange-correlation functional and pseudopotentials were Perdew–Burke–Ernzerhof Generalized Gradient Approximation and projector-augmented-wave potentials [30–32], respectively. A cutoff energy of 750 eV was used for the structural optimization and band structure calculations, with Monkhorst-Pack k -mesh densities of $2\pi \times 0.02 \text{ \AA}^{-1}$ [33]. The superconducting properties of the dynamically stable compounds were further investigated using quantum espresso (QE) [34]. The electron-phonon coupling calculations were carried out via QE with ultrasoft pseudopotentials, with a kinetic energy cutoff of 60 Ry and a k -point mesh spacing of $2\pi \times 0.02 \text{ \AA}^{-1}$ [35]. The corresponding q mesh was set to $2\pi \times 0.04 \text{ \AA}^{-1}$. The predicted T_c values were estimated by directly solving the isotropic Migdal–Eliashberg equation using the elk code [36] with the Coulomb pseudopotential μ^* set to a typical value of 0.1.

III. RESULTS AND DISCUSSION

In this work, we performed geometry optimizations of more than 462 ternary structures based on the prototype of $P6/mmm\text{-LaSc}_2\text{H}_{24}$. Metal elements from Groups I–IV of the periodic table (including La, Ce, Ac, and Th) were used to occupy the La and Sc sites in all possible permutations. Among them, 21 structures were identified as dynamically stable at 300 GPa, including the previously reported $\text{LaSc}_2\text{H}_{24}$ and $\text{ThY}_2\text{H}_{24}$ (Table I), for which we evaluated their T_c values. The results revealed that $\text{LaSc}_2\text{H}_{24}$, $\text{ThY}_2\text{H}_{24}$, and $\text{AcSc}_2\text{H}_{24}$ all exhibit T_c values exceeding 273 K (0 °C). In contrast,

TABLE I. Superconducting properties of dynamically stable compounds at 300 GPa. T_c values were evaluated using the isotropic Eliashberg equation with $\mu^* = 0.1$.

Compound	$\omega_{\log}$	λ	T_c (K)
ThY ₂ H ₂₄	1161	2.39	300
LaSc ₂ H ₂₄	839	2.57	286
AcSc ₂ H ₂₄	983	2.64	276
ZrMg ₂ H ₂₄	783	2.68	267
CaZr ₂ H ₂₄	586	3.02	262
ThCa ₂ H ₂₄	530	2.96	250
KTi ₂ H ₂₄	595	2.68	215
CeCa ₂ H ₂₄	951	1.97	206
CeMg ₂ H ₂₄	901	1.66	203
AcHf ₂ H ₂₄	1326	1.46	198
AcZr ₂ H ₂₄	1333	1.46	197
LaZr ₂ H ₂₄	1375	1.41	195
ThSc ₂ H ₂₄	1584	1.29	194
LaHf ₂ H ₂₄	1374	1.34	187
CeSc ₂ H ₂₄	1572	1.14	164
ThHf ₂ H ₂₄	1462	1.06	148
LaTh ₂ H ₂₄	953	1.12	113
CeHf ₂ H ₂₄	1428	0.88	108
CeZr ₂ H ₂₄	1500	0.85	107
CeTh ₂ H ₂₄	1132	0.39	4
ThCe ₂ H ₂₄	1164	0.35	2

CeTh₂H₂₄ and ThCe₂H₂₄ exhibit much lower T_c values of 4 and 2 K, respectively, highlighting the significant variations in superconducting behavior within this structural framework. It is worth noting that through stability analysis, most of these compounds are not thermodynamically stable at 300 GPa and become dynamically unstable as the pressure decreases to 250 GPa. Nevertheless, these compounds provide valuable superconducting data that contribute to the clathrate superconductor database and enable in-depth investigation into the underlying superconducting mechanisms. Therefore, in this study, we focus solely on their superconducting properties for model development and mechanistic analysis.

Most of the structures exhibit T_c values exceeding 200 K, suggesting that this framework holds significant potential for high-temperature superconductivity. Taking ThY₂H₂₄, the

compound with the highest predicted T_c , as an example, the ELF analysis reveals a metallic hydrogen network, with the shortest H-H distances ranging from approximately 1.0 to 1.35 Å. The ELF values exceed 0.5 between hydrogen atoms, indicating metallic bonding characteristics, which are typical features of clathrate superhydrides (Fig. 2). Band structure calculations further confirm the strong metallicity of these compounds. At the Fermi level, the density of states is primarily derived from hydrogen atoms. Figure 2 presents the distribution of T_c values along with their corresponding PDOS_H values. Generally, T_c and PDOS_H show a consistent correlation, with a Pearson correlation coefficient of 0.75. However, as shown in Fig. 2, within the T_c range of 200–260 K, the trend in T_c variation differs from that of PDOS_H. Additionally, LaTh₂H₂₄ shows significant fluctuations in PDOS_H, suggesting that superconducting performance may be influenced by factors beyond the electronic properties.

We further conducted a detailed structural analysis and identified three specific compounds of LaTh₂H₂₄, CeTh₂H₂₄, and ThCe₂H₂₄, where the B-site elements belong to lanthanide and actinide metals. Due to their relatively large atomic radii, these elements induce an expansion of the surrounding hydrogen cages, leading to a transition of the hydrogen network from a three-dimensional to a two-dimensional configuration (see Supplemental Material Fig. S1 [37] for the distribution of hydrogen bonds), which consequently weakens the electron-phonon coupling (EPC). Calculations of the electron-phonon coupling coefficient (λ) reveal that CeTh₂H₂₄ and ThCe₂H₂₄ exhibit λ values of less than 0.4, while LaTh₂H₂₄ has a λ of 1.12. In contrast, LaSc₂H₂₄, which shares a similar PDOS_H value with LaTh₂H₂₄, exhibits a significantly higher λ of 2.57, representing a 56% reduction in LaTh₂H₂₄ compared to LaSc₂H₂₄. To quantify the impact of hydrogen bond length modifications induced by metal atoms, along with electronic structure, on the EPC strength, we propose an empirical parameter $\tilde{S}_{\text{couple}}$, as defined in Eq. (1). This parameter incorporates ELF_m, the average ELF value of H-H bonds, and bonds_m, the mean bond length of all hydrogen bonds within the unit cell. The results demonstrate a strong correlation between $\tilde{S}_{\text{couple}}$ and λ (correlation coefficient = 0.91), as well as T_c (0.87), as shown in Fig. 3, surpassing the correlation between PDOS_H and T_c . Interestingly, $\tilde{S}_{\text{couple}}$ shows only a weak correlation of 0.42 with PDOS_H, suggesting that it captures

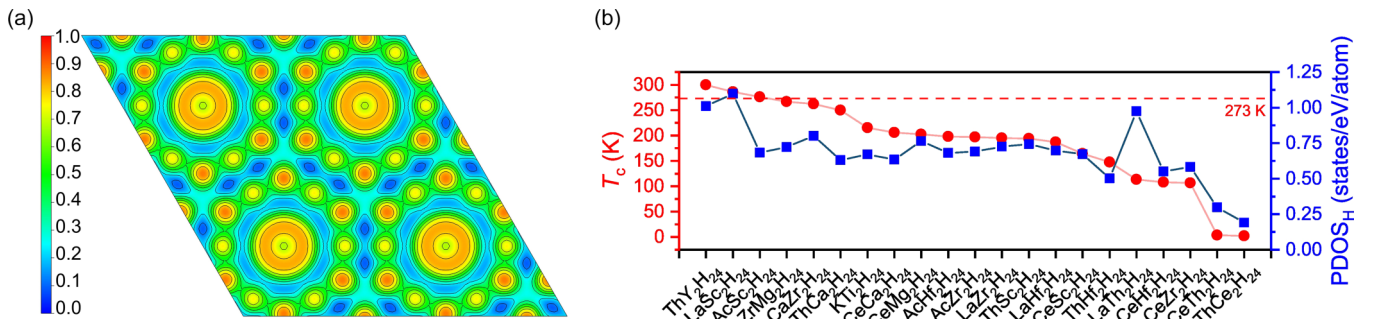


FIG. 2. (a) The ELF isosurface of $P6/mmm$ -ThY₂H₂₄ at 300 GPa along the (0,0,1), showing that 12 hydrogen atoms form an extensive metallic network. (b) Distribution of the predicted superconducting transition temperatures (T_c , red circles) and the corresponding hydrogen-projected density of states at the Fermi level (PDOS_H, blue squares) for AB₂H₂₄-type compounds. The red dashed line marks 273 K as a reference point for room temperature.

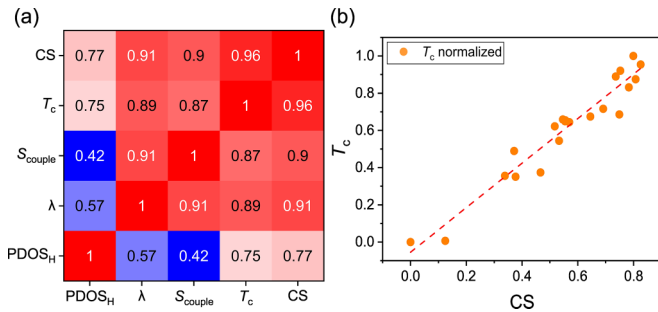


FIG. 3. (a) Correlation heat map illustrates the pairwise correlation of T_c , S_{couple} , λ , PDOS_H, and CS. The color scale indicates the strength of correlations. (b) Scatter plot showing the linear relationship between the normalized values of T_c and the combined descriptor CS, demonstrating a clear positive correlation that captures the underlying superconducting trends within the AB_2H_{24} framework.

essential physical factors influencing EPC strength beyond conventional electronic properties.

Furthermore, by considering both PDOS_H and $\bar{S}_\text{couple}$ in relation to T_c , we performed a linear fit and introduced an additional empirical parameter, CS, as defined in Eq. (2). This combined parameter exhibits an even stronger correlation with T_c , reaching a correlation coefficient of 0.93, indicating that CS provides a more comprehensive measure of the key factors governing superconductivity (Fig. 3). The regression coefficients in the CS model can be interpreted as the relative weights of the constituent parameters, indicating that PDOS_H and $\bar{S}_\text{couple}$ contribute approximately equally to T_c . These results suggest that $\bar{S}_\text{couple}$ effectively captures the underlying physical mechanisms of superconductivity. The corresponding numerical data are provided in Table S1.

$$\overline{S}_{\text{couple}} = \text{ELF}_m \times \text{bonds}_m, \quad (1)$$

$$\text{CS} = 0.46\text{PDOS}_{\text{H}} + 0.54\bar{S}_{\text{couple}}. \quad (2)$$

Building on the parameter model derived from the AB_2H_{24} dataset, it is of great interest to evaluate its generalizability and predictive capability across other clathrate-type hydride superconductors. Our analysis shows that the two proposed parameters can be effectively extended to additional systems, including ternary compounds such as $Li_2MH_{16/17}$ and binary superhydrides like MH_6 , MH_9 , and MH_{10} , through a minor modification to Eq. (1) incorporating an appropriate weighting correction.

This correction is essential, as restricting the analysis to the AB_2H_{24} system would overlook the diversity of hydrogen bond length distributions across different structural frameworks. In such cases, using simple average ELF values and bond lengths fails to accurately capture the underlying superconducting behavior. Therefore, we conducted a comprehensive analysis in the space of hydrogen bond length and T_c values across all considered frameworks, as illustrated in Fig. 4(a). The top panel of Fig. 4(a) shows the distribution of H-H bond lengths within the range of 0.85–1.30 Å. The color intensity represents the associated T_c strength for each bond length, with deeper red denoting higher T_c values. Hydrogen bonds longer than 1.05 Å tend to positively contribute to T_c , whereas those shorter than 1.0 Å exhibit negligible impact. The bottom panel of Fig. 4(a) presents the normalized contribution of bond lengths to T_c , obtained by dividing the cumulative T_c by the number of bonds at each corresponding length. The resulting distribution exhibits a Gaussian-like profile, with a prominent peak near 1.07 Å, suggesting that hydrogen bonds of this length most effectively enhance superconductivity. To incorporate this trend into S_{couple} , we introduce a Gaussian-weighted correction function $W(i)$ to modify Eq. (1), yielding the weighted S_{couple}^w as presented in Eq. (3). The $W(i)$ is constructed based on the distribution of bond lengths and their respective contributions within the superconducting framework. It is defined as $1 + G(c1, s1) - G(c2, s2)$, where i denotes the length of hydrogen bonds and G represents a Gaussian function. The shape of the weighting function is illustrated by the blue curve in

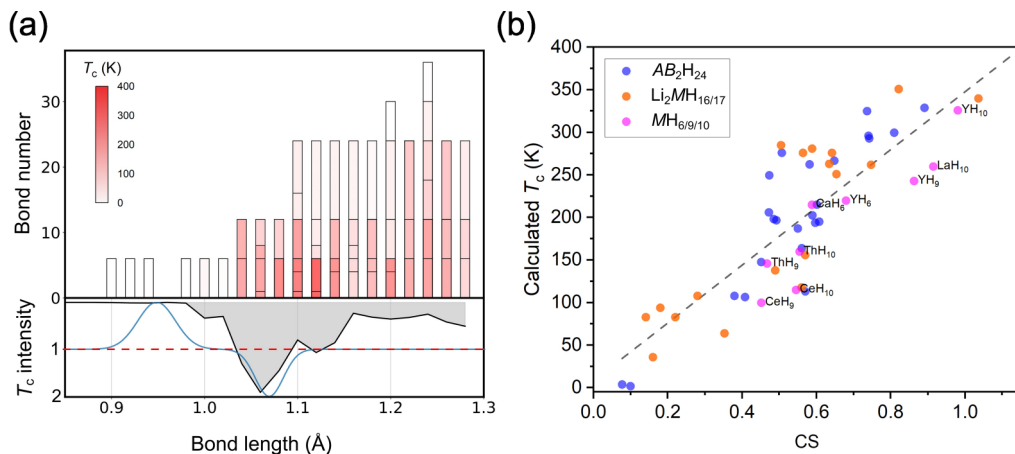


FIG. 4. (a) The top panel illustrates the distribution of hydrogen bond counts with respect to bond length. The intensity of red color indicates the magnitude of T_c values, based on data from AB_2H_{24} , $Li_2MH_{16/17}$, MH_6 , MH_9 , and MH_{10} systems. The bottom panel presents the normalized contribution of bond lengths to T_c , revealing a prominent peak around 1.07 Å, indicating that hydrogen bonds of this length most effectively enhance superconductivity. The blue curve represents the weighting function $W(i)$ introduced in the revised S_{couple} parameter. (b) Scatter plot showing the linear correlation between the revised CS parameter and the calculated T_c across all considered clathrate superconductors.

the lower panel of Fig. 4(a). This function comprises two components: a reward term for bond lengths near 1.07 Å and a penalty term for bonds shorter than 1.0 Å, where no contribution to T_c is observed. The four hyperparameters, $c1$ and $c2$ (centers), and $s1$ and $s2$ (standard deviations), were optimized using a grid search algorithm and determined to be 1.07, 0.95, 0.015, and 0.02, respectively.

$$S_{\text{couple}}^w = \sum_i W(i) \times \text{ELF}(i) \times \text{bonds}(i). \quad (3)$$

The final unified CS parameter, applicable across AB_2H_{24} , $Li_2MH_{16/17}$, MH_6 , MH_9 , MH_{10} systems, is presented in Eq. (4). The fitting performance is shown in Fig. 4(b). The correlation coefficients between T_c and PDOS_H , T_c and S_{couple}^w , and T_c and CS are 0.70, 0.60, and 0.85, respectively. When evaluated within individual systems, the correlation between T_c and CS reaches 0.86 for $Li_2MH_{16/17}$ and 0.93 for $MH_{6/9/10}$. Meanwhile, the correlation between S_{couple}^w and PDOS_H is only 0.18. These results confirm that CS serves as a robust and system-independent descriptor for superconducting performance in clathrate hydrides. The low correlation between S_{couple}^w and PDOS_H further suggests these parameters capture distinct aspects of the electronic structure and bonding environment. Overall, the weighted model offers a powerful framework for understanding the superconducting mechanisms in diverse hydride systems.

$$\text{CS} = 0.51\text{PDOS}_H + 0.49S_{\text{couple}}^w. \quad (4)$$

Previous studies have investigated the correlation between the properties of hydride superconductors and their T_c values by constructing empirical descriptors. For instance, Belli *et al.* proposed the Φ_{DOS} descriptor, which integrates the highest value of ELF isosurface, the fraction of hydrogen atoms, and the density of states (DOS), demonstrating consistent performance across various hydrogen-based superconductors [23]. Building on this, Ma *et al.* enhanced the model performance for binary clathrate superhydrides by introducing the AE parameter, defined as the average ELF value within the structure [38]. The modified model achieved satisfactory performance for systems such as MH_6 , MH_9 , and MH_{10} . However, the limited variability of hydrogen-bonding environments in binary hydrides restricts the applicability of such models to ternary clathrates, where H-H interactions are significantly more diverse. In our previous work, we proposed the E_{couple} descriptor to improve the generalizability across clathrate hydride superconductors by incorporating both DOS and H-H bond information [21]. However, its formulation lacked clear physical interpretability, as it was derived via symbolic regression methods. In this work, we address these limitations by introducing physically intuitive descriptors that integrate DOS, ELF, and H-H bond characteristics. By aggregating the contributions of individual H-H bonds through a weighted summation, the proposed model exhibits improved

robustness across complex clathrate frameworks. Furthermore, by explicitly decomposing T_c into two independent components, PDOS_H and S_{couple} , our approach offers a concise and interpretable framework for understanding superconductivity in high-pressure hydrides.

IV. CONCLUSION

In summary, we systematically investigated the superconducting properties of $P6/mmm\text{-}AB_2H_{24}$ clathrate hydrides by analyzing more than 462 compounds at 300 GPa. Our calculations identified 21 dynamically stable compounds, with predicted T_c values ranging from 2 to 300 K. Through detailed structural and electronic analysis, we introduced two empirical descriptors, S_{couple} and CS, to elucidate the correlations of superconducting behavior, structural features, and electronic properties. We found that different metal elements influence superconductivity through two key mechanisms: donating electrons to hydrogen atoms at the Fermi level and modifying the hydrogen metallic network through size effects, thereby affecting the EPC strength. Furthermore, our parameter model can be extended to other clathrate-type hydride systems, such as $Li_2MH_{16/17}$ and binary superhydrides (MH_6 , MH_9 , and MH_{10}). By incorporating an additional weighting function, we significantly enhanced the model's generalizability. This extension further underscores the effectiveness of the S_{couple} descriptor, as the weighting function offers intuitive insight into how variations in hydrogen bond lengths influence T_c values. When applied to the full dataset, the refined CS descriptor achieves a strong correlation coefficient of 0.85, demonstrating robust predictive capability across diverse structural systems. The proposed descriptors, S_{couple} and CS, provide a practical framework for evaluating key factors governing superconducting behavior and for predicting T_c values. These findings lay a foundation for the rational design of high-temperature superconductors in hydrogen-rich materials.

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DATA AVAILABILITY

No data were created or analyzed in this study.

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