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First-Principles Investigation of Structural, Electronic, X-ray Spectroscopic, and Optical Properties of $CaRhH_3$

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ABSTRACT

The $CaRhH_3$ compound has recently attracted attention due to its potential application in hydrogen energy systems; however, its electronic and optical properties remain insufficiently explored. In this work, density functional theory (DFT) calculations within the CASTEP framework are employed to systematically investigate the structural, electronic, and optical characteristics of $CaRhH_3$. Structural stability is confirmed through full geometry optimization and simulated powder X-ray diffraction analysis. The calculated electronic band structure indicates metallic behavior, primarily governed by Rh-d states near the Fermi level. To enhance the reliability of the electronic structure analysis, Gaussian Process Regression (GPR)-based machine learning is applied to the density of states (DOS), enabling smooth profile generation and uncertainty quantification. This approach significantly improves peak identification and interpretation of electronic features. Furthermore, element-specific X-ray absorption and emission spectrum provide detailed insight into the contributions of Ca and Rh to the occupied and unoccupied states. Optical properties, including absorption and reflectivity, reveal strong interaction with electromagnetic radiation, particularly in the ultraviolet region. This study highlights the methodological novelty of integrating DFT with machine learning techniques for advanced electronic structure analysis. The findings not only improve the fundamental understanding of $CaRhH_3$ but alswo demonstrate its potential suitability for hydrogen energy applications, offering both scientific and technological significance.

INTRODUCTION

There has been significant research interest in hydrogen materials, in particular transition metal hydrides, owing to the increasing demand for clean energy on a global platform (Dewangan *et al.*, 2022). It has been widely recognized that hydrogen-rich materials possess suitable properties for energy conversion materials, hydrogen storage, and catalysis due to the abundance of hydrogen in these materials (Saad & Myat, 2025). Metal hydrides are promising candidates for the development of complex functional materials because of the favorable properties they display due to metal-hydrogen interactions (Cuevas *et al.*, 2022; El Kharbachi *et al.*, 2020; Xu *et al.*, 2024). Because of their partially filled d-orbitals, which lead to greater metal-hydrogen interactions, there has been considerable interest in the field of transition metal hydrides (McGrady & Guilera, 2003). The optical properties, reactivity, and electrical conductivity of the material are greatly affected by metal-hydrogen interactions. Alkaline earth metals, when used in conjunction with transition metal hydrides, often help in the creation of materials that possess variable physical properties along with better structural stability (Pearson, 1985; Saad). In such materials, the role of the transition metal is mostly limited to the regulation of the electronic properties and the type of chemical bonding, whereas the other metal acts as the electropositive element. Owing to the wide range of physical properties as well as flexibility in crystal structure, the hydride structures related to perovskites are a material of prime significance. The importance of these hydride structures largely arises from the flexibility in crystal structure that allows scientists to precisely change the composition of these materials to tailor their electric properties. There are various transition metal hydrides of calcium that are still not properly understood in the context of the current renewed interest in metal hydrides. Calcium is a preferred element due to its highly desirable chemical and mechanical properties and is therefore widely used in many forms for energy applications (Oganov *et al.*, 2019; Schneemann *et al.*, 2018). Moreover, even though rhodium is a noble transition metal with high catalytic activity and prominent d-state contributions, these can be expected to make a notable difference to the overall electronic structure and bonding properties for hydrides. As such, it is believed to behave in a manner that is quite unique for the $CaRhH_3$ system regarding its metallic electric properties and overall electronic features with structural stability. However, the literature is still to be supplemented with theoretical work that focuses on the electric and optical properties of the material in question $CaRhH_3$ (Aldridge & Downs, 2001; Yuan *et al.*, 2024).

Density functional theory, or DFT, first-principal calculations have been a trustworthy and acknowledged approach for the atomic-level intrinsic properties research for crystal materials. The CASTEP approach, which is characterized as a plane-wave basis set approach together with a pseudopotential approach, as one of the first-principles calculations, has been commonly

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adopted as a method among those tools provided for the precise determination of structural, electrical, or optical properties within transition-metal hydrides (Hasnip *et al.*, 2014; Rahman). Some result outputs, such as density-of-states outputs, could involve numerical noises, which may leave minute details essential for precise determination, even though DFT calculations offer abundant microscopic details. The integration of first-principal calculations and methods from machine learning as well as artificial intelligence has proven to be a very successful approach in the last few years to enhance data analysis, visualization, as well as uncertainty estimation. Gaussian Process Regression (GPR) is a method which also has a probabilistic learning framework that allows precise reconstruction of smooth electronic spectra and estimation of confidence intervals to communicate uncertainty estimates in predictions (Arfi *et al.*, 2025; Lin *et al.*, 2014). All these features are highly valuable in density-of-states calculations, where the location as well as magnitude determination of peaks accurately matters a lot to interpret electrical properties.

In this study, a combination of Artificial Intelligence (AI) and Machine Learning techniques with respect to Gaussian Process Regression has been incorporated with Density Functional Theory calculations to analyze $CaRhH_3$ (Jin *et al.*, 2022; Lin *et al.*, 2014). Simulated Powder X-ray diffraction techniques and thorough geometry optimization studies have helped to analyze the structure quality and stability. The results obtained from electronic band structure calculations along with Density of States analyses helped to analyze the electronic properties of $CaRhH_3$. The electronic properties of $CaRhH_3$ can now be analyzed with more accuracy using the artificial intelligence-based method incorporated in this study, which has enhanced peak identification reliability and spectral clarity. The analysis of the X-ray absorption and emission spectroscopy of the given elemental structure helps better comprehend the role of Ca and Rh atoms. The role of these atoms, as stated, can be better explored with the help of optical properties such as absorbance and reflectivity. The combined analysis of the DFT and AI (Artificial Intellegece) model of the current study helps establish the significance of $CaRhH_3$ material in the domain of hydrogen energy technology while presenting a contemporary perspective of the material.

MATERIALS AND METHODS

Computational Methodology

All calculations done in this study employed the density functional theory approach with the CASTEP module of the Materials Studio simulation package (Basri *et al.*, 2015; Jin *et al.*, 2022). Core-valence interactions were accounted for with ultrasoft pseudopotentials. This approach has a good compromise between computational speed and precision. The Perdew-Burke-Ernzerhof functional with generalized gradient approximation was employed to describe the exchange-correlation functional (Adedoja *et al.*, 2023). A plane wave with a cutoff of 580 eV was employed in the study. This ensures convergence of the total energy and the electronic structures. The Monkhorst-Pack k-point mesh was chosen to be fine enough to ensure the convergence of the total energy calculations in the Brillouin zone integration. The BFGS algorithm was used in structural relaxation (Adedoja *et al.*, 2023). Both the lattice parameters and the atomic positions were fully relaxed until the convergence criteria were satisfied for the total energy, the components of the interatomic forces, the stress components, and the atomic displacements. When the change in the total energy became smaller than 1.0×10^{-2} eV per atom, the self-consistent field (SCF) calculations were judged to be converged. After the X-R-M---R path, the electronic band structure calculation was carried out along the high-symmetry lines in the Brillouin zone after completion of the geometry optimization process. With a higher k-point mesh and the Fermi level as the zero-reference level, the density-of-states calculation was performed to yield smooth and accurate spectral results. Moreover, for understanding element-specific electronic transition properties, X-ray absorption spectra (XAS) and X-ray emission spectra (XES) calculations were carried out at the Ca and Rh K-edges, respectively. The above spectra give a qualitative understanding of the occupied as well as the unoccupied electronic levels. These were obtained based on the calculated electronic structure. The complex dielectric function was employed in the framework of linear response theory to investigate the optical properties of the $CaRhH_3$ compound. The calculation of the optical properties was carried out in such a way as to ensure the energy resolution is fine enough to warrant the correct treatment of the optical transitions.

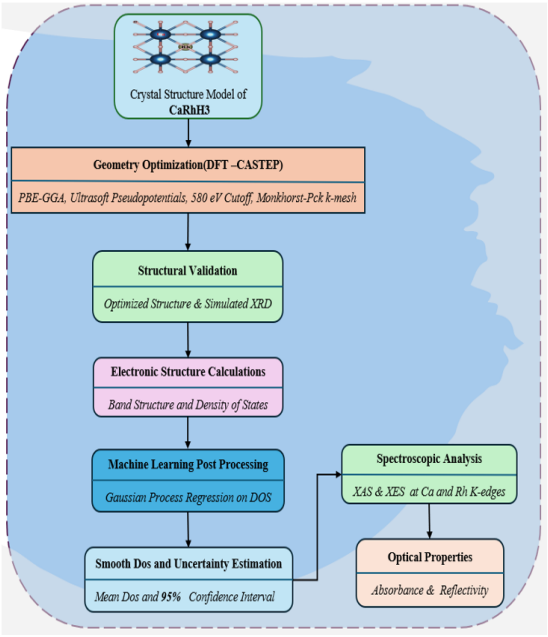

Figure 1: Computational workflow adopted for the structural, electronic, spectroscopic, and optical analysis of $CaRhH_3$.

Gaussian Process Regression Analysis

GPR was then used as a Machine-Learning-based (ML) post-processing technique to generate a smooth and physically meaningful DOS (Giannakis *et al.*, 2019). The discrete DOS results from the first-principles calculations were used as the training dataset, with the DOS values as the output target and energy levels as the input variable. To model these smooth transitions in electronic structure data, a squared exponential, also called a radial basis function, kernel was used (Akbar *et al.*, 2025). To ensure a balanced level of adaptability and prevent overfitting, the GPR model was trained using maximum likelihood to search for hyperparameter values. The density of states, as a smooth function, is captured from the GPR mean function, while the corresponding 95% confidence band reflects how uncertain predictions were made across the energy ranges (Akbar *et al.*, 2025). Although it retains the original physical phenomenon modeled in the density functional theory, it makes possible efficient noise reduction, enhanced definition of the peaks, and better visibility of the electrical properties.

RESULTS AND DISCUSSION

Structural Properties

Using the CASTEP tool within Materials Studio and a cutoff plane wave energy of 580 eV (Troullier & Martins, 1991), $CaRhH_3$ crystal structure and corresponding $CaRhH_3$ structural stability were explored and the workflow shown in Figure 1. As shown in Figure 2(a), $CaRhH_3$ in a fully relaxed state displays a remarkably clear crystal structure where Ca and Rh cations form a uniformly distributed crystal structure. Although Ca cations form a corner of a crystal structure and hence offer $CaRhH_3$ structural stability through anionic interactions, Rh cations form a hydrogen ring and hence a strong metallic hydrogen component. $CaRhH_3$ clearly displays a high degree of structural stability under my simulation settings. A precise account of electronic interactions in Ca, Rh, and H atoms has been provided by the high cutoff energy value, which further helps in obtaining correct results for the calculation of the total energy of optimized systems. High Rh and H interaction values are very important for maintaining a structure framework, which has its own uniqueness in being a transition-metal hydride complex. Figure 2(b) reveals the X-ray diffraction pattern obtained from the optimized structure. The high degree of crystallinity in the $CaRhH_3$ phase is evident in its sharp and clear diffraction peaks in this pattern. The characteristic lattice planes in their cubic crystal structure are associated with specific peaks appearing at $2\theta = 32°$ and 35°. The absence of other peaks indicates a favorable structure in the optimized arrangement and confirms the formation of a single-phase material (Li *et al.*, 2025). The relatively large atomic factor for Rh, an essential component in understanding the diffraction profile, is the driving force behind the intensity variations in the diffraction peaks. Regarding the upcoming experimental synthesis of $CaRhH_3$, the above simulation of the XRD profiles will serve as a point of comparison. Finally, the simulation diffraction data, along with the optimized crystal shape, confirm that $CaRhH_3$ is indeed a hydride with high structural stability, while it could also serve as an appropriate material for further property analysis concerning electric, mechanical, and energy properties due to the high metal–hydrogen bonding network present in the compound. Figure 2 (a) The optimized crystal structure of $CaRhH_3$ and the corresponding simulated X-ray diffraction pattern were obtained using the CASTEP code; distribution and location of Ca and Rh atoms in the lattice. The black and grey balls denote Ca and Rh atoms, respectively. (b) The simulated XRD pattern of the fully relaxed crystal structure.

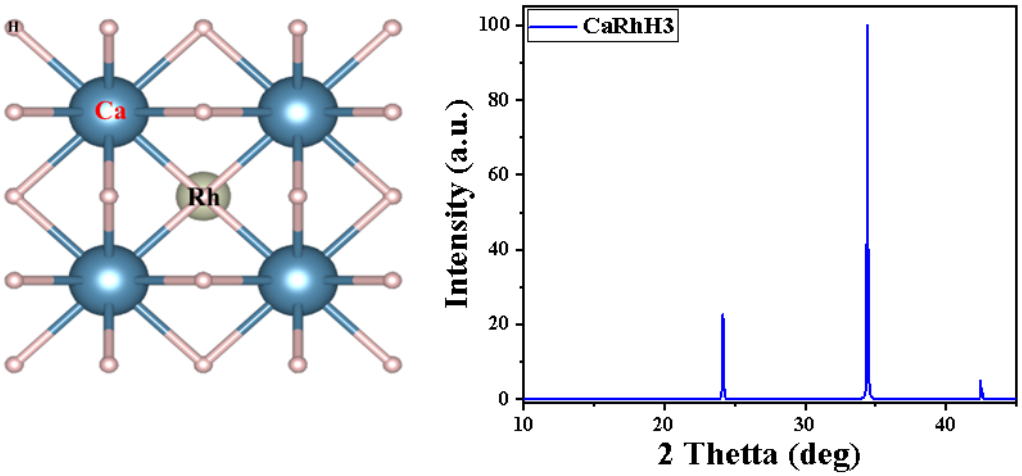

Figure 2: Optimized crystal structure and simulated X-ray diffraction pattern of $CaRhH_3$ obtained using the CASTEP code. (a) Cation arrangement in the optimized crystal structure, highlighting the distribution of Ca and Rh atoms within the lattice. (b) Simulated XRD pattern calculated from the fully relaxed structure.

Electronic Properties

Castep module of Materials Studio was employed in density functional theory calculation to assess the $CaRhH_3$ crystal structure and its electrical properties identified $CaRhH_3$ with stable cubic structure evenly dispersed with Ca and Rh ions as depicted in Figure 2(a). While the Ca ions are responsible for the stabilization of the lattice through ionic bonds, the other metal ions (Rh) were found to be evenly surrounded by the hydrogen atoms, thus stabilizing the lattice through metal-hydrogen bonds (Zhang *et al.*, 2023) as can be seen in Figure 3 (a). Moreover, the $CaRhH_3$ has no lattice distortion when the system is optimized as indicated in the figures below: Figure 3 (b) verifies good crystalline quality and phase purity of $CaRhH_3$, which has clear diffraction peaks and no signature of impurities. As Figure 3. reveals, the density of states and the electronic band structures were employed to investigate the electronic structure of $CaRhH_3$. $CaRhH_3$ can be metallic because the total density of states has a finite density of states at the Fermi level, which has been set to zero at 0 eV. In this case, the Rh d-states dominate the Fermi level while the H-related states reside at lower energy levels; therefore, Rh-H bonding has high probability. As there are many bands that cross the Fermi level in the vicinity of the highly symmetrical points (X, R, M, and back to R) in the Brillouin zone, the band structure of Figure 3(b) indicates the metallic property of $CaRhH_3$. The dispersiveness of the bands at or near the Fermi level assures highly mobile carriers of the charge, which ensures the applicability of the material with regard to the requirement for efficient metal conductivity (Pan *et al.*, 2022; Zhang *et al.*, 2025). It can be inferred that the obtained compound has appreciable metal-hydrogen bonding and metallic property. It has the potential to be used for hydrogen-related applications.

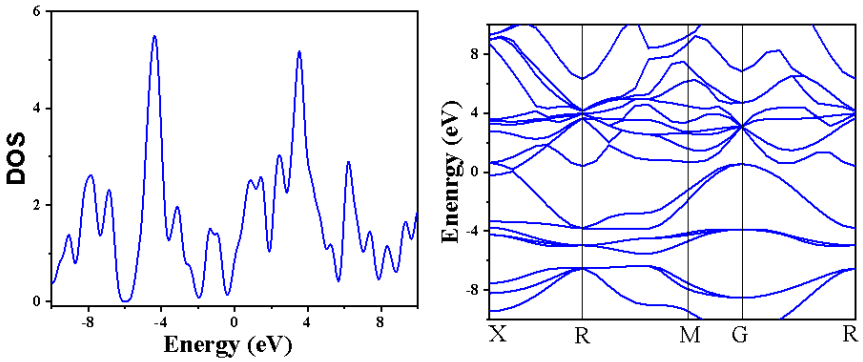

Figure 3: The electronic properties of $CaRhH_3$ calculated by the CASTEP algorithm. (a) The total density of states represented as a function of the energy, where the Fermi level is considered as 0 eV. (b) The high-symmetry paths of the Brillouin zone correspond to the band structure of $CaRhH_3$.

X-ray Absorption and Emission Spectra

The nature of the element-specific electronic structure and bonding features was further probed by investigating the X-ray absorption and emission properties of $CaRhH_3$ (Kerr *et al.*, 2022; Khan *et al.*, 2023). Figure 4(a) shows the calculated X-ray absorption spectra at the Ca and Rh K-edges. The particular absorption features in the case of Ca and Rh originate due to electronic transitions from core levels to unoccupied states above the Fermi level. The stronger and broader absorption profile of the Rh K-edge as compared to Ca reflects the greater contribution of the Rh d-states to the conduction area and their strong hybridization with hydrogen orbitals. A more ionic character of Ca within the host lattice is represented through the relatively sharper nature of its absorption spectrum at the K-edge. This is consistent with the role of Ca as an electropositive element that has a primarily supporting role in charge stabilization

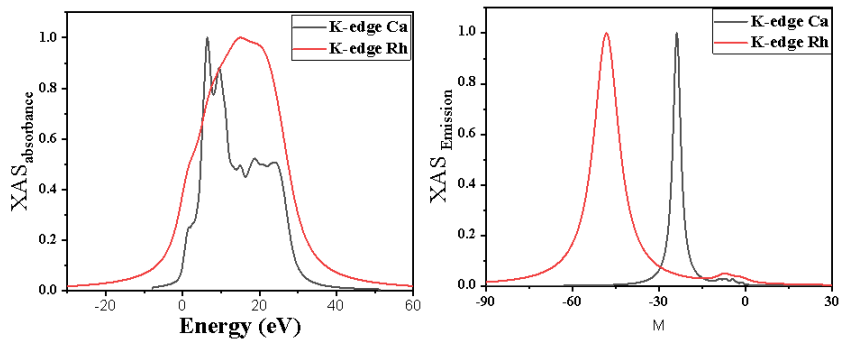

Figure 4: Calculated X-ray emission and absorption spectra of $CaRhH_3$. (a) XAS taken at the Rh and Ca K-edges. (b) XES related to the Ca and Rh K-edges, highlighting the element-specific electronic states and the associated underlying electronic transitions.

overactive electronic conduction (Liu *et al.*, 2024). The occupied electronic states are identified via the associated X-ray emission spectra (XES), which are shown in Figure 4(b). The dominant intensity of the Rh K-edge emission attributable to the transitions involving the occupied Rh d-states is further affirmation of the relatively less dominant role of Ca states near the Fermi level (Khan *et al.*, 2024). This is attributed by the wider distribution of the Ca K-edge emission. The XAS and XES analysis elucidates that Rh significantly influences the electronic structure of the $CaRhH_3$ compound, with Ca having a supporting role via ionic interactions. These results confirm the metallic character of $CaRhH_3$ and point out the strong hybridization of metal and hydrogen states within the host lattice. They also support the DOS and band structure studies as mentioned earlier.

Optical Properties

To gain better insight into the interaction of $CaRhH_3$ with electromagnetic radiation, as well as to assess its potential optoelectronic properties, the optical properties of $CaRhH_3$ were studied (Shu *et al.*, 2025). Figure 5(a) presents the calculated optical absorbance as a function of the wavelength. Due to the transition of electrons from the occupied valence energy levels to the unoccupied levels with higher energies, there is a prominent absorbance in the ultraviolet region, cakes 300 nm. There is a progressive reduction in absorbance with an increase in wavelength towards the visible and near-infrared regions, representing a lower extent of photon absorption at lower energies (Han *et al.*, 2024). The existence of electronic states at the Fermi level is revealed by the sustained absorbance within the visible part of the spectrum, which is reflected by the metallicity of $CaRhH_3$ discussed on the basis of the band structure. Apparently, such phenomena indicate that interband transitions contribute considerably to the optical properties of the material. In Fig.4(b), the optical reflectivity of $CaRhH_3$ with varying photon energy is illustrated. Much reflection is observed in the low energy part with notable peaks, while the highest peak in the medium energy band can be noticed. These properties can be attributed mainly to interband transitions and the presence of collective electrical excitations. There is a sharp drop in the reflection of light when the photon energy is increased, thus suggesting an increase in the absorption of photons.$CaRhH_3$ has moderate values of reflectivity for low energy values and a considerable level of absorbance in the UV region, based on a broad assessment of absorbance and reflectivity values. The properties highlighted above make $CaRhH_3$ a potentially

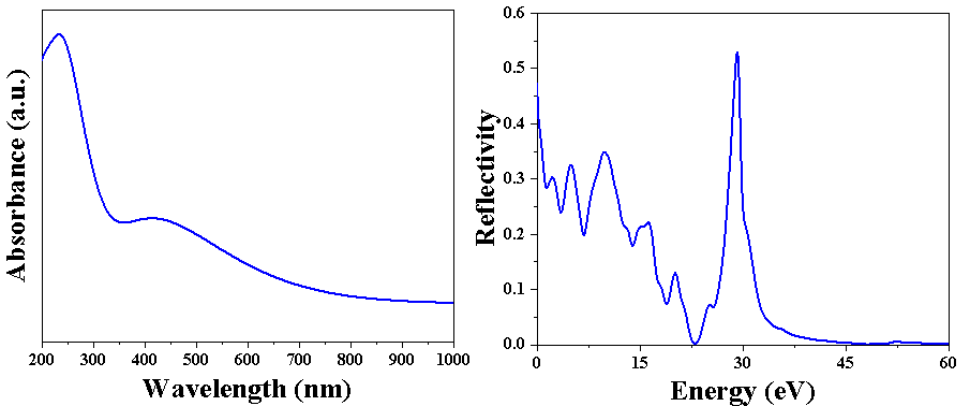

Figure 5: Shows the calculated optical properties of $CaRhH_3$. (a) Optical absorbance variation with wavelength in the 200–1000 nm range.

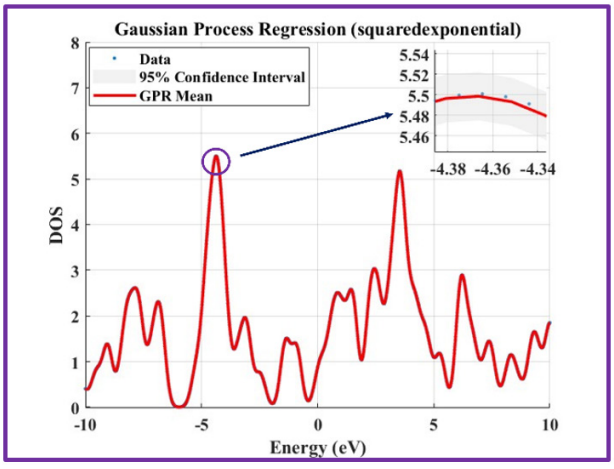

Figure 6: Gaussian Process Regression (GPR) of the density of states (DOS) versus Energy.

useful material in terms of applications in UV protection, optoelectronics, and energy-related areas.

An artificial intelligence (AI) and machine learning (ML) technique of Gaussian Process Regression was then used to investigate the density of states, which were obtained through these first-principle calculations (El-Adawy *et al.*, 2024). Figure 1 shows the computational workflow for the spectroscopic and optical studies of $CaRhH_3$, density functional theory calculations, and machine learning-based (ML) density of states analysis. DOS profile reconstructed using Gaussian Process Regression as shown in Figure 6. The mean curve from the GPR model tracks the original data points reasonably well, which indicates that the adopted regression approach effectively captures the key features of the electronic structure (Afrasiabi, 2023). The shaded band corresponding to the 95% confidence interval remains narrow for most of the energy range, which reflects a high level of confidence in the model's predictions (Stahl *et al.*, 2023). A distinct DOS peak around -4.4 eV is given by the enlarged inset, and the sharp feature is accurately retained by the GPR model, with a smooth reproduction showing the ability of the squared exponential kernel to catch the localized electronic states. Simultaneously, the GPR curve does not develop unwanted oscillations while maintaining the proper peak positions and relative intensities, both very important for a reliable interpretation of the electronic behavior (Vanguri *et al.*, 2022). Furthermore, within regions where data points are few, the width of the uncertainty interval expands slightly, thereby reflecting how the model itself is aware of the inadequacy of data in such regions. Also, the computation of the standard deviation of uncertainty clearly reveals regions where more data should be sampled.

CONCLUSION

In the current work, the $CaRhH_3$ structural, electronic, and optical properties were carefully investigated utilizing first-principles density-functional calculations in an artificial intelligence-assisted analysis. Geometric optimization and simulated X-ray diffraction analysis confirmed the $CaRhH_3$ stability and clear crystalline character. Based on analysis of the electronic band structure and density of states calculation, it was revealed that $CaRhH_3$ behaves like a metal with predominant Rh d-orbital character close to the Fermi level, which reflects high metal and H states hybridization. The Gaussian Process Regression tool represented a reliable and Data-driven method of post-processing the Density of States, allowing uncertainty analysis and seamless Spectrum reconstruction without altering the original DFT outcomes. Specifically, in regions of energies characterized by sharp and highly localized states, this tool improved Peak resolution and facilitated analysis of electrical behavior. Moreover, the analysis of optical properties revealed substantial Absorption in the ultraviolet region accompanied by Moderate reflection values, while X-ray Absorption and Emission Spectra allowed element-specific information of the electronic properties to be gained through Spectroscopy. It is evident from this research that the integration of machine learning approaches, such as GPR, with first-principles calculations is an accurate and trustworthy approach for the complex analysis of electrical structures in a given material. Not only is there an appropriate understanding about the properties of $CaRhH_3$, but it also encompasses a novel tool for the development of additional research in the approach to hydrogen energy materials.

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