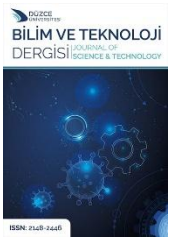

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Research paper

Hydrogen-Driven Perpendicular Magnetic Anisotropy at the Co/Ir Interface

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ABSTRACT

Magnetic anisotropy at the nanoscale is a key property for developing advanced spintronic devices, information storage systems, and gas sensors. In this study, we investigate the hydrogen-assisted perpendicular magnetic anisotropy (PMA) in the Co/Ir interface through first-principles density functional theory calculations. Initially, the Co/Ir system exhibits in-plane magnetic anisotropy (IMA). Upon hydrogen absorption, a significant increase in magnetic anisotropy energy is observed, indicating a transition from IMA to PMA. This behavior contrasts sharply with the Co/Rh system, where hydrogen absorption leads to a reduction in magnetic anisotropy energy and a switch from PMA to IMA. The underlying mechanism of these transitions is linked to the hybridization of atomic orbitals at the interface. These findings highlight the potential of hydrogenation as a tool to reversibly control magnetic anisotropy in Co/Ir interfaces, paving the way for new applications in spintronics and gas sensing technologies.

Keywords: *Perpendicular Magnetic Anisotropy, Hydrogen Absorption, Density Functional Theory (DFT), Spintronics*

I. INTRODUCTION

Magnetic anisotropy is a fundamental property of magnetic materials, as it defines the preferred direction of magnetic moments and governs the dynamics of magnetization switching (Klyukin et al., 2020; Hellman et al., 2017; Capku et al., 2020). The ability to tune magnetic anisotropy plays a crucial role in the development of advanced technologies, including spintronic devices, magnetic storage systems, and sensors (Dieny & Chshiev, 2017). Among the various types, perpendicular magnetic anisotropy (PMA) has attracted significant interest due to its relevance in high-density magneto-optical storage and spintronic applications (Dieny & Chshiev, 2017; Bauer et al., 2015; Deger et al., 2019; Deger, 2020a). Recent research has revealed that the magnetic properties of thin films and heterostructures can be significantly altered by introducing light elements such as hydrogen. This process, termed magneto-ionics, enables the ionic manipulation of magnetic behavior via ion movement, leading to notable modifications in the electronic structure of materials (Maruyama et al., 2009; Bi et al., 2014; Erkovan et al., 2022). In particular, hydrogen has been shown to affect magnetic anisotropy in several ferromagnetic/nonmagnetic (FM/NM) interfaces, rendering it an attractive candidate for energy-efficient, reversible magnetization control (Hsu et al., 2018; Munbodh et al., 2012; Deger, 2020b).

The interaction between hydrogen and magnetic interfaces can either enhance or suppress PMA, depending on the material system and hydrogen concentration. For instance, in Co/Pd interfaces, hydrogen tends to accumulate at the interface, leading to a reduction in PMA and a transition to in-plane magnetic anisotropy (IMA) (Munbodh et al., 2012; Causer et al., 2019). Conversely, in Fe/V systems, hydrogen

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promotes PMA, illustrating the tunability of hydrogen-induced magnetic effects (Hsu et al., 2018; Broddefalk et al., 2002). These results demonstrate that hydrogenation is a promising approach to modulating magnetic anisotropy; however, the mechanisms underlying these effects are complex and highly dependent on the specific system (Okabayashi et al., 2018; Chang et al., 2013). The Co/Ir interface is of particular interest in the context of hydrogen-assisted magnetic anisotropy due to its strong spin-orbit coupling, which can induce PMA under suitable conditions (Yang et al., 2015; Demiroglu et al., 2024). While Co/Pd and Co/Pt interfaces have been widely studied due to their robust PMA and extensive experimental verification, the Co/Ir interface remains relatively underexplored. This is primarily due to its more complex electronic structure and less conventional magnetic behavior, which are strongly influenced by Ir's high spin-orbit coupling. These unique characteristics position Co/Ir as a promising candidate for achieving reversible control of magnetic anisotropy through hydrogenation, potentially surpassing the performance of conventional Co/Pd or Co/Pt systems in spintronic and magneto-ionic applications. Despite this potential, the influence of hydrogen absorption on the magnetic anisotropy of Co/Ir interfaces has not been comprehensively studied. Understanding how hydrogen alters the magnetic characteristics of this system may provide insights for designing spintronic components and magnetic sensors with tunable anisotropy (Bauer et al., 2015; Gilbert et al., 2016; Sisman et al., 2024; Harumoto et al., 2025).

In this work, we explore the impact of hydrogen absorption on the magnetic anisotropy of Co/Ir and Co/Rh interfaces using first-principles density functional theory (DFT) calculations. Our results indicate that the Co/Ir system initially exhibits IMA, but undergoes a transition to PMA upon hydrogenation. This transition is driven by hydrogen-induced hybridization of atomic orbitals at the interface. Interestingly, this mechanism contrasts with that observed in Co/Rh and Co/Pd systems. The findings presented here deepen our understanding of hydrogen-controlled magnetic phenomena and highlight the potential of hydrogenated FM/NM interfaces for future information processing, data storage, and sensing technologies.

II. MATERIAL AND METHOD

The perpendicular magnetic anisotropy (PMA) calculations were performed using the constrained spin method, implemented within the Vienna Ab-initio Simulation Package (VASP) (Kresse & Hafner, 1993; Kresse & Furthmüller, 1996). This method has previously been applied in various studies for calculating the Dzyaloshinskii–Moriya interaction (DMI), including in bulk frustrated systems, insulating chiral-lattice magnets, and ferromagnetic/heavy metal (FM/HM) interfaces (Xiang et al., 2011; Yang et al., 2015; Zhang et al., 2018; Soumyanarayanan et al., 2017). To account for electron-electron interactions, we employed the Generalized Gradient Approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) functional (Perdew et al., 1996; Perdew et al., 2008). Electron-ion interactions were treated using the projector augmented wave (PAW) method (Kresse & Joubert, 1999). The plane-wave energy cutoff was set to 400 eV. The face-centered cubic (fcc) crystal structures were oriented along the (111) direction. To prevent interactions between periodic images, an 8-monolayer (ML) thick vacuum slab was introduced along the out-of-plane (z) direction. Brillouin zone integration was performed using a Γ-centered Monkhorst-Pack grid of 4×4×1, ensuring sufficient convergence. Structural relaxation was performed until the residual atomic forces were less than 1 meV/Å, and the electronic self-consistency criterion was set to 10^{-5} eV in total energy. The hydrogen migration barriers presented in Figure 2 were calculated using the nudged elastic band (NEB) method as implemented in VASP. Intermediate images between the initial and final states were generated to map the minimum energy path, and all atomic positions were relaxed perpendicular to the reaction coordinate. In our NEB calculations, a single hydrogen atom per unit cell was introduced at the most stable adsorption site on the Rh and Ir layers..

After relaxation, electronic charge distributions were calculated by solving the Kohn–Sham equations without spin–orbit coupling. Subsequently, two spin configurations (perpendicular and in-plane) were constructed using the constrained spin method (Yang et al., 2015). In the constrained spin method, the spin quantization axis is fixed along specific crystallographic directions (in-plane and out-of-plane) during total energy calculations. The magnetic anisotropy energy (MAE) is then determined as the total energy difference between these two spin orientations in the presence of spin–orbit coupling.

III. RESULTS AND DISCUSSIONS

The process of hydrogen absorption in Rh-Ir/Co systems plays a crucial role in modifying the magnetic anisotropy of the system. Figure 1 provides a schematic illustration of how hydrogen atoms interact with a bilayer system consisting of a Rh/Ir layer (orange spheres) and a Co layer (blue spheres). The figure demonstrates the progressive stages of hydrogen atom absorption and its potential influence on the

system's electronic and magnetic properties. Here, in panel (a), hydrogen atoms (red spheres) begin to approach the surface of the Rh/Ir layer. At this initial stage, the Co and Rh/Ir layers are not yet significantly influenced by hydrogen, and the system retains its original configuration. As hydrogen atoms begin to penetrate the Rh/Ir layer in panel (b), the interaction between hydrogen and the electronic structure of the Rh/Ir layer intensifies, potentially altering the electronic distribution and initiating a change in the system's magnetic properties. Finally, in panel (c), hydrogen atoms have become embedded within the Rh/Ir layer, forming stable interactions with the underlying atomic structure. This is a conceptual framework for understanding how hydrogen absorption might induce changes in the material's overall properties. These changes could include modifications to magnetic anisotropy, which will be explored in subsequent results. The absorption process visualized here highlights the potential of hydrogen to act as a tunable factor in adjusting the magnetic properties of Rh/Ir-Co bilayer systems.

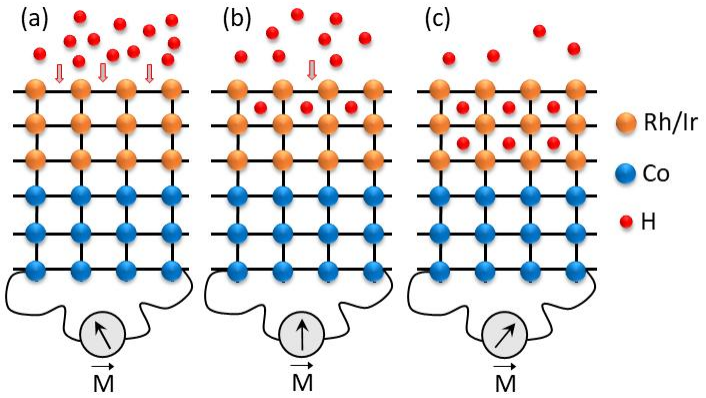

Figure 1. Schematic illustration of the hydrogen absorption process in Rh/Ir-Co bilayer systems. The panels depict the different stages of hydrogen interaction with the Rh/Ir layer and how this interaction potentially alters the overall electronic and magnetic properties of the system. Hydrogen atoms penetrate the Rh/Ir layer, leading to structural changes that may influence the magnetic anisotropy of the Co layer.

Hydrogen migration plays a critical role in determining how effectively it can be absorbed into materials and subsequently influence their magnetic properties. Figure 2 shows the calculated energy barriers for hydrogen migration into the Rh and Ir layers, providing key insights into the energy required for hydrogen atoms to penetrate these two materials. The vertical axis represents the relative energy (in electron volts), while the horizontal axis corresponds to the path coordinate, which tracks the progression of hydrogen through the Rh or Ir layer. The magenta and orange lines represent the energy barrier for Rh and Ir, respectively. We observed a clear difference in the energy barriers for hydrogen absorption between the two systems. For Rh, the energy barrier peaks at approximately 2.1 eV, indicating that hydrogen absorption into Rh requires relatively higher energy input. In contrast, the energy barrier for Ir is lower, with a maximum around 1.8 eV, suggesting that hydrogen atoms can more easily penetrate the Ir layer compared to Rh. This difference in energy barriers implies that hydrogen absorption into the Ir layer is more favorable, which could lead to faster and more efficient changes in the magnetic and electronic properties of the Co/Ir system compared to Co/Rh. The comparison between Rh and Ir in this figure is particularly important for understanding how hydrogen absorption affects the magnetic properties of the Co layer in the corresponding Co/Rh and Co/Ir bilayers. This finding emphasizes the role of the underlying material (Rh or Ir) in controlling the interaction between hydrogen and the bilayer system, which is crucial for designing materials with tunable magnetic properties.

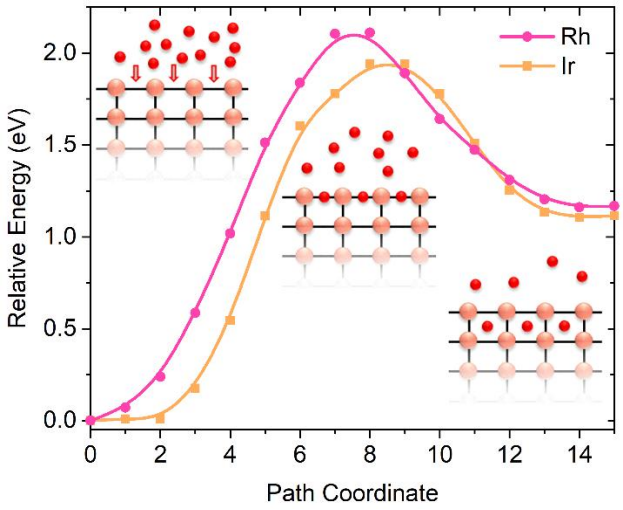

Figure 2. Energy barriers for hydrogen migration into the Rh and Ir layers. The path coordinate on the horizontal axis represents the progression of the hydrogen atom as it moves through the lattice of the Rh or Ir layer, starting from the surface and progressing into the material. This coordinate helps track the energy changes the hydrogen atom experiences during its migration into the system, highlighting the distinct energy barriers in each layer.

Figure 3 illustrates the effect of hydrogen absorption on the magnetic anisotropy energy (MAE) in Co/Rh and Co/Ir bilayer systems. The vertical axis shows the magnetic anisotropy energy (in meV/atom), while the horizontal axis represents the different system configurations, including Co/Rh and Co/Ir before and after hydrogen absorption. Positive values on the MAE axis indicate perpendicular magnetic anisotropy (PMA), while negative values indicate in-plane magnetic anisotropy (IMA). The first two bars in the figure represent the magnetic anisotropy energy of the Co/Rh and Co/Ir systems before hydrogen absorption. For Co/Rh, the MAE is positive, indicating a preference for perpendicular magnetic anisotropy. In contrast, the Co/Ir system shows a negative MAE, suggesting that the system initially favors in-plane magnetic anisotropy. These initial differences between the two systems can be attributed to the intrinsic properties of the Rh and Ir layers, with Rh supporting PMA and Ir promoting IMA under these conditions (Lau et al., 2019; Aksu et al., 2020). Upon hydrogen absorption (represented by the bars to the right of the vertical dashed line), both systems undergo significant changes in their magnetic anisotropy energy. For the Co/Rh system, hydrogen absorption causes a reduction in MAE, ultimately leading to a switch from PMA to IMA. This suggests that the hydrogen atoms disrupt the interaction responsible for perpendicular anisotropy, pushing the system toward an in-plane configuration. On the other hand, the Co/Ir system shows the opposite effect: hydrogen absorption significantly increases the MAE, resulting in a transition from IMA to PMA. This behavior indicates that hydrogen stabilizes the perpendicular magnetic configuration in the Co/Ir system, effectively reversing the initial in-plane preference. The contrasting behavior of the two systems upon hydrogen absorption highlights the tunable nature of magnetic anisotropy in these bilayers. While Co/Rh loses its perpendicular anisotropy and transitions to an in-plane state, Co/Ir gains perpendicular anisotropy with the introduction of hydrogen. This finding is particularly significant for applications where control over magnetic anisotropy is crucial, such as in spintronic devices or magnetic sensors. By selectively incorporating hydrogen into these systems, it may be possible to reversibly switch between PMA and IMA, providing a flexible tool for tuning magnetic properties in multilayered structures. While these changes in magnetic anisotropy are evident, a deeper understanding of the electronic structure modifications responsible for these transitions requires an analysis of the density of states.

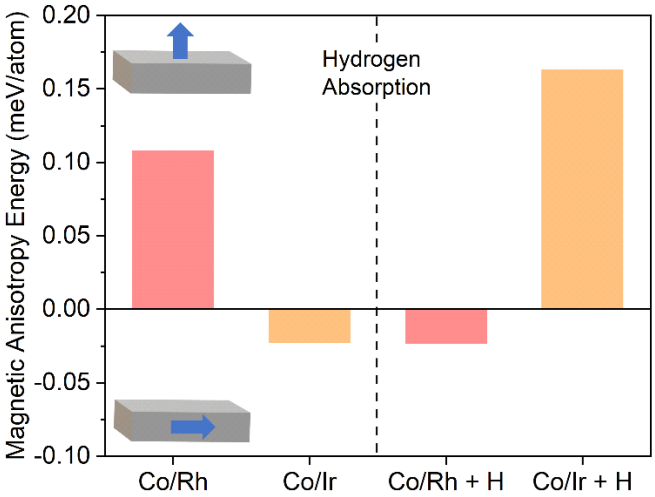

Figure 3. Magnetic anisotropy energy (MAE) before and after hydrogen absorption in Co/Rh and Co/Ir systems. The positive MAE values indicate perpendicular magnetic anisotropy (PMA), while negative values indicate in-plane magnetic anisotropy (IMA). Hydrogen absorption causes a transition from PMA to IMA in Co/Rh, whereas in Co/Ir, it induces a switch from IMA to PMA, demonstrating the tunability of magnetic anisotropy via hydrogen absorption.

Figure 4 presents the density of states (DOS) for the Co/Rh and Co/Ir bilayer systems, both before and after hydrogen absorption, providing deeper insight into the electronic structure changes that drive the observed magnetic anisotropy shifts. Panels (a) and (b) represent the Co/Rh system before and after hydrogen absorption, respectively, while panels (c) and (d) show the corresponding results for the Co/Ir system. In panel (a), the DOS of the Co/Rh system before hydrogen absorption indicates a significant degree of hybridization between the Co (blue) and Rh (pink) states near the Fermi level. This hybridization is critical in stabilizing the perpendicular magnetic anisotropy observed in Figure 3, as the electronic structure supports a strong interaction between the two layers (Deger, 2020b). However, after hydrogen absorption (panel b), the hybridization between Co and Rh is disrupted, particularly around the Fermi level. This disruption weakens the interaction that favors PMA, leading to a reduction in the magnetic anisotropy energy and a transition to in-plane magnetic anisotropy, as shown in Figure 3. For the Co/Ir system, panel (c) shows that, before hydrogen absorption, there is limited hybridization between the Co (blue) and Ir (orange) states near the Fermi level. This lack of hybridization corresponds to the in-plane magnetic anisotropy observed in Figure 3. However, after hydrogen absorption (panel d), significant hybridization between Co and Ir states emerges near the Fermi level. This newly formed hybridization stabilizes the perpendicular magnetic anisotropy, causing the system to transition from IMA to PMA. The DOS analysis presented in Figure 4 thus provides a clear explanation for the changes in magnetic anisotropy energy observed in Figure 3. In the Co/Rh system, hydrogen disrupts the hybridization that supports PMA, leading to a switch to IMA. Conversely, in the Co/Ir system, hydrogen promotes hybridization, which in turn stabilizes PMA. The hydrogen-induced changes in MAE can be understood in the context of spin–orbit coupling and orbital moment anisotropy. Hydrogenation modifies the local electronic environment at the Co/Ir interface, enhancing the hybridization between Co and Ir states near the Fermi level. This enhanced hybridization strengthens SOC interactions and alters orbital moment anisotropy, both of which contribute to the stabilization of perpendicular magnetic anisotropy in the hydrogenated Co/Ir system. These findings highlight the pivotal role of electronic structure changes in governing the magnetic properties of bilayer systems and underscore the potential of hydrogen as a tunable factor in modulating magnetic anisotropy.

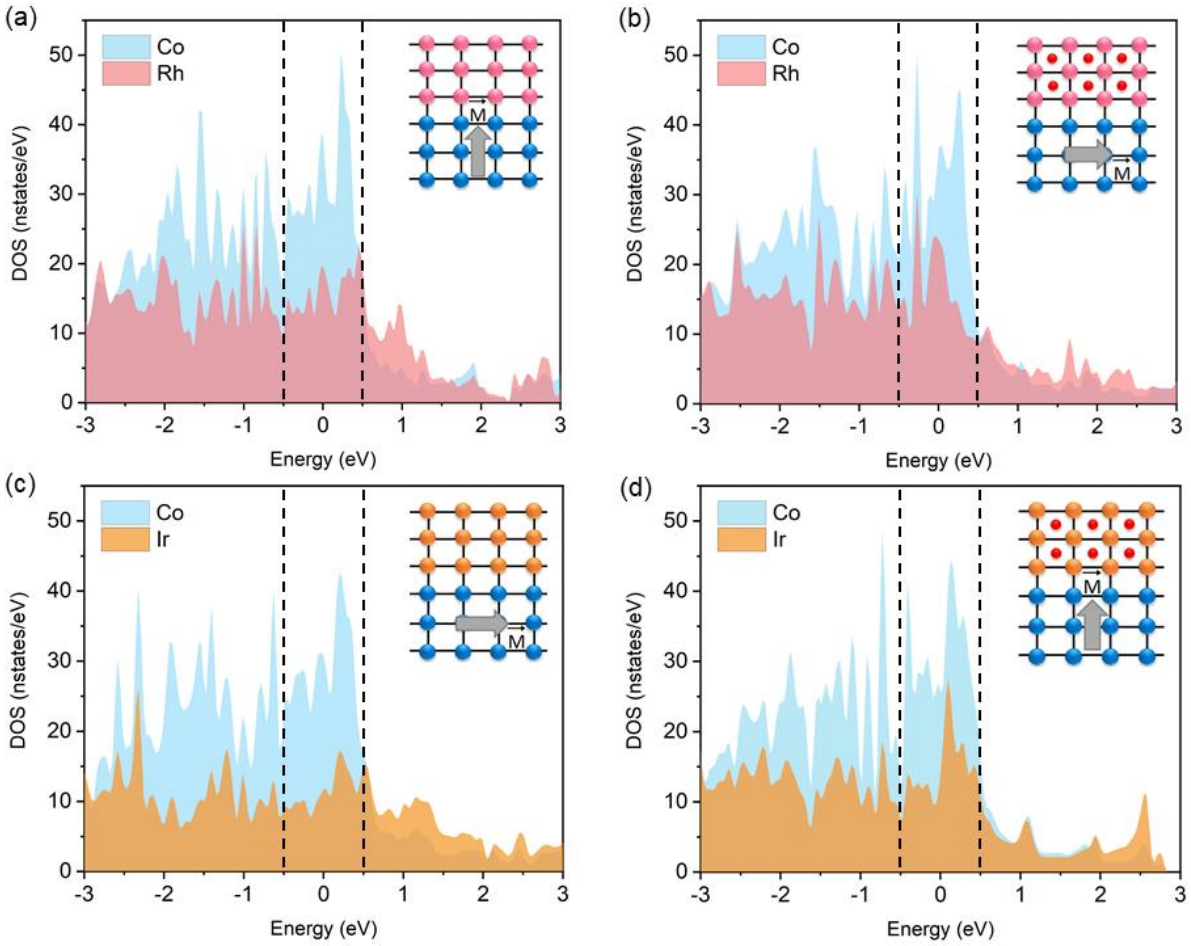

Figure 4. Density of states (DOS) for Co/Rh and Co/Ir systems, both before and after hydrogen absorption. Panels (a) and (b) represent the DOS for the Co/Rh system before and after hydrogen absorption, respectively. Panels (c) and (d) show the DOS for the Co/Ir system before and after hydrogen absorption, respectively. In panels (a) and (b), the blue and pink areas respectively represent the DOS contribution from Co and Rh layers. In panels (c) and (d), the blue and yellow areas represent the DOS contribution from Co and Ir atoms, respectively. The DOS reveals that hydrogen absorption disrupts the hybridization in Co/Rh, weakening the perpendicular magnetic anisotropy, while in Co/Ir, it induces hybridization, stabilizing the perpendicular configuration.

The results of this study demonstrate that hydrogen absorption plays a pivotal role in modulating the magnetic anisotropy in Co/Rh and Co/Ir bilayer systems. The observed transition from perpendicular magnetic anisotropy to in-plane magnetic anisotropy in the Co/Rh system upon hydrogen absorption aligns with findings from previous studies on similar systems. For instance, Munbodh et al. (2012) demonstrated that hydrogen absorption into Co/Pd multilayers reduces PMA, leading to an in-plane anisotropy, suggesting that the underlying mechanism of hydrogen disrupting hybridization at the interface is consistent across multiple systems (Munbodh et al., 2012). Similarly, hydrogen-induced transitions in magnetic anisotropy have been reported in Co/Pt systems, where hydrogen's role in weakening the orbital hybridization between layers explains the loss of PMA (Causer et al., 2019). This study is the first to demonstrate that hydrogen absorption can induce perpendicular magnetic anisotropy in such systems. The discovery of this hydrogen-assisted perpendicular magnetic anisotropy marks a significant advancement in the understanding of tunable magnetic properties. Such a system holds great promise for applications in spintronic devices, particularly in magnetic data storage and retrieval processes, where precise control over magnetic anisotropy is essential. These findings pave the way for innovative approaches to magnetic writing and reading technologies in next-generation spintronic applications.

IV. CONCLUSION

In this study, we investigated the effect of hydrogen absorption on the magnetic anisotropy of Co/Rh and Co/Ir bilayer systems using first-principles calculations. Our findings revealed that hydrogen plays a

critical role in modulating the magnetic properties of these systems. For the Co/Rh system, hydrogen absorption disrupts the initial hybridization between the Co and Rh layers, leading to a decrease in magnetic anisotropy energy (MAE) and a transition from perpendicular magnetic anisotropy (PMA) to in-plane magnetic anisotropy (IMA). In contrast, for the Co/Ir system, hydrogen absorption induces hybridization between Co and Ir, stabilizing the perpendicular magnetic configuration and driving a transition from IMA to PMA. The density of states (DOS) analysis provided a clear understanding of these transitions, demonstrating that the underlying electronic structure changes are responsible for the observed magnetic anisotropy shifts. These results underscore the tunability of magnetic properties through hydrogen absorption and highlight the potential of Co/Ir bilayer systems for applications in spintronics and magnetic sensors, where control over magnetic anisotropy is essential. These computational findings can serve as a guideline for experimental studies aiming to validate hydrogen-mediated PMA in Co/Ir interfaces. Furthermore, this approach could be extended to more complex multilayer structures and other FM/NM interfaces, offering pathways for designing advanced spintronic and magneto-ionic devices. The reversible nature of the hydrogen-induced transitions offers new opportunities for designing next-generation devices with adjustable magnetic characteristics.

DECLARATIONS

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Conflict of Interest Disclosure: The author declares no conflict of interest.

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Plagiarism Statement: This article has been evaluated for plagiarism and no instances of plagiarism were detected.

Availability of Data and Materials: Data sharing is not applicable to this study.

Use of AI Tools: AI-assisted tools were used only to improve the language clarity and readability of the manuscript. The author takes full responsibility for the final content.

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