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Exploring Distinct Materials for Hydrogen Storage: A Density Functional Theory Approach

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Abstract : Developing efficient hydrogen storage materials is critical to advancing clean energy technologies, particularly for applications in fuel cells and renewable energy systems. This study explores materials for hydrogen storage through Density Functional Theory (DFT) calculations, addressing one of the most significant challenges in sustainable energy: the safe and efficient storage and release of hydrogen. Our research provides an in-depth analysis of various candidate compounds' structural and electronic properties, aiming to identify materials with enhanced hydrogen storage capacities. By investigating adsorption mechanisms and optimizing key material properties, we aim to contribute to developing high-performance hydrogen storage solutions. The findings from this work have the potential to impact the field of hydrogen fuel technology significantly, offering insights and advancements that support the transition to sustainable energy systems.

Keywords : hydrogen storage, density functional theory, electronic, thermal stability
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