First-Principles Study of Hydrogen Adsorption on Metal-Decorated SnS_2 and $SnSe_2$ Monolayers under Electric Fields

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The global transition toward sustainable energy has positioned hydrogen as a promising clean energy carrier[1], offering high gravimetric energy density and water as its only byproduct[2]. However, safe, efficient, and scalable hydrogen storage remains a major challenge. Conventional methods—such as high-pressure tanks and cryogenic storage—pose safety risks and high energy costs, limiting their practicality for large-scale deployment.[3] These challenges have driven intensive research into solid-state hydrogen storage materials, which offer a more stable and compact alternative.

In this study, we investigate hydrogen adsorption on SnS_2 and $SnSe_2$ monolayers decorated with alkali (Li, Na, K) and alkaline-earth (Mg, Ca) metals using first-principles density functional theory (DFT) calculations. Our results reveal that metal decoration significantly enhances hydrogen adsorption, with Ca-decorated SnX_2 (X = S, Se) exhibiting the strongest binding and highest hydrogen uptake. We further analyze temperature, pressure, and external electric field effects to assess practical viability. Our findings indicate that higher pressures improve adsorption stability, with desorption temperatures approaching the operational limits of proton exchange membrane (PEM) fuel cells (~233 K). An external electric field (~–0.5 V/Å) also strengthens hydrogen binding, offering a tunable strategy to optimize storage performance.

These results highlight the potential of metal-decorated SnX_2 monolayers as promising hydrogen storage materials. Further optimization strategies— co-doping, defect engineering, and electric field tuning—could help advance these materials toward practical applications in sustainable hydrogen energy systems.

References

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