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Comparative Computational Study of Semi-Metallic Zintl Hydrides for Hydrogen Storage Applications

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ABSTRACT

Efficient, safe, and compact solid-state materials are critical for overcoming hydrogen storage challenges. This study introduces a novel class of materials, the hexagonal Zintl-phase hydrides SnMSiH (M = Al, Ga), and establishes their exceptional potential through first-principles density functional theory (DFT) calculations. The key superiority of these materials lies in their unique semimetallic electronic structure, which significantly enhances hydrogen interactions by reducing the activation energy for desorption, enabling efficient and reversible cycling—a critical improvement over insulating or wide-bandgap hydrides. Structurally, the primitive hexagonal framework (space group P3m1) provides optimal diffusion pathways for hydrogen. We report a high gravimetric capacity of 0.58 wt% for SnAlSiH with a near-ambient desorption temperature of 310.69 K, markedly superior to many complex hydrides. SnGaSiH offers a capacity of 0.47 wt% at an even lower desorption temperature of 254.15 K, indicating easy hydrogen release. Thermodynamically, both compounds exhibit significant thermal expansion and high heat capacities, ensuring resilience at operating temperatures. Mechanically, they are highly anisotropic; SnAlSiH's higher compressibility may facilitate volume changes during cycling, while SnGaSiH demonstrates superior mechanical stability (higher elastic constants). This combination of favorable desorption thermodynamics, intrinsic structural stability, and robust mechanical properties distinguishes SnMSiH hydrides as premier candidates for application. This work provides a foundational strategy for further performance enhancement through alloying and defect engineering.

1 | Introduction

Energy generation has been a fundamental aspect of human civilization for centuries. However, the increasing reliance on fossil fuels has led to environmental concerns and the depletion of hydrocarbon resources. Several alternative energy sources have been explored to mitigate greenhouse gas emissions and reduce dependence on fossil fuels [1, 2]. The global pursuit of sustainable energy is driven by multiple factors, including political pressures from energy-importing nations, environmental concerns linked to the Kyoto Protocol, and the declining availability of petroleum reserves [3]. As a response to these challenges, hydrogen-based energy has emerged as a promising solution [4]. Unlike hydrocarbons,