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First-Principles Thermodynamics and Kinetics of Advanced Hydrogen Storage Materials¹

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Hydrogen-fueled vehicles require a cost-effective, light-weight material that binds hydrogen strongly enough to be stable at ambient pressures and temperatures but weakly enough to liberate H₂ with minimal heat input. Since none of the simple metal hydrides satisfy all the requirements for a practical H₂ storage system, recent research efforts have turned to complex hydrides and advanced multicomponent material compositions. We will show that first-principles density-functional theory (DFT) calculations have become a valuable tool for understanding and predicting novel hydrogen storage materials. Recent studies in our group have used DFT calculations to (i) predict crystal structures of new solid-state hydrides, (ii) determine phase diagrams and thermodynamically favored reaction pathways in multinary hydrides, and (iii) study microscopic kinetics of diffusion, phase transformations, and hydrogen release.

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