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First-Principles Thermodynamics and Kinetics of Advanced Hydrogen Storage Materials[1]

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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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