First Principles predictions of Hydrogen Storage Materials

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A grand challenge in materials technology is the development of materials capable of reversible storage of $\text{H}_2$ at ambient temperatures and pressures capable of mass densities greater than 6% by weight. We report here the results of first principles calculations on several classes of materials including:

- Carbon-alkali based systems
- Metal oxide framework systems
- Metal alloy systems.

These simulations indicate that the DOE goals for 2010 are achievable in materials that could be manufactured today.

\(^1\)In collaboration with Weiqiao Deng, Caltech