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First Principles predictions of Hydrogen Storage Materials[1]

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A grand challenge in materials technology is the development of materials capable of reversible storage of 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