



## Developing hydrogen storage materials with DFT

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**Abstract:** With oil reserves slated to be greatly diminished as soon as 50 years from now, it is imperative to plan a transition to an alternative energy carrier. One ideal candidate is hydrogen, which produces energy through its reaction with oxygen, the only byproduct being water. Unfortunately, alongside a couple of other significant practical barriers, hydrogen gas has far too low density (by volume) to be practical for automotive use, one of the most significant sources of petroleum consumption. Condensing pure hydrogen, while useful for prototype hydrogen vehicle, does not yield the desired storage densities or energy efficiency to be competitive with petroleum, so the Department of Energy has been focusing efforts on studying solid hydrogen storage materials, which can ideally achieve greater densities than compressing hydrogen alone. In this presentation, I will review work I've done using density functional theory to study three different hydrogen storage materials.