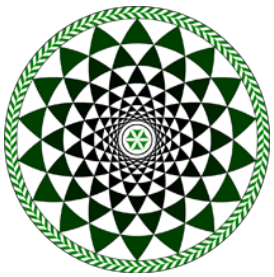

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Challenges in theoretical description of molecular crystals for energy storage

Tuesday, July 7, 2015 3:30 PM (20 minutes)

Metal borohydride complexes and their derivatives are of great interest due to their potential as hydrogen storage materials. Thermodynamic and kinetic properties of these materials can be tuned using: mixed-metal borohydride complexes; ammonia-containing metal borohydrides; confinement of these materials in small nanopores. Any of such procedures leads to materials with complex crystalline structure that is difficult to study due to large fraction of light elements.
Challenges in theoretical description of tuned complex hydrides will be presented.

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