

Poster Presentation

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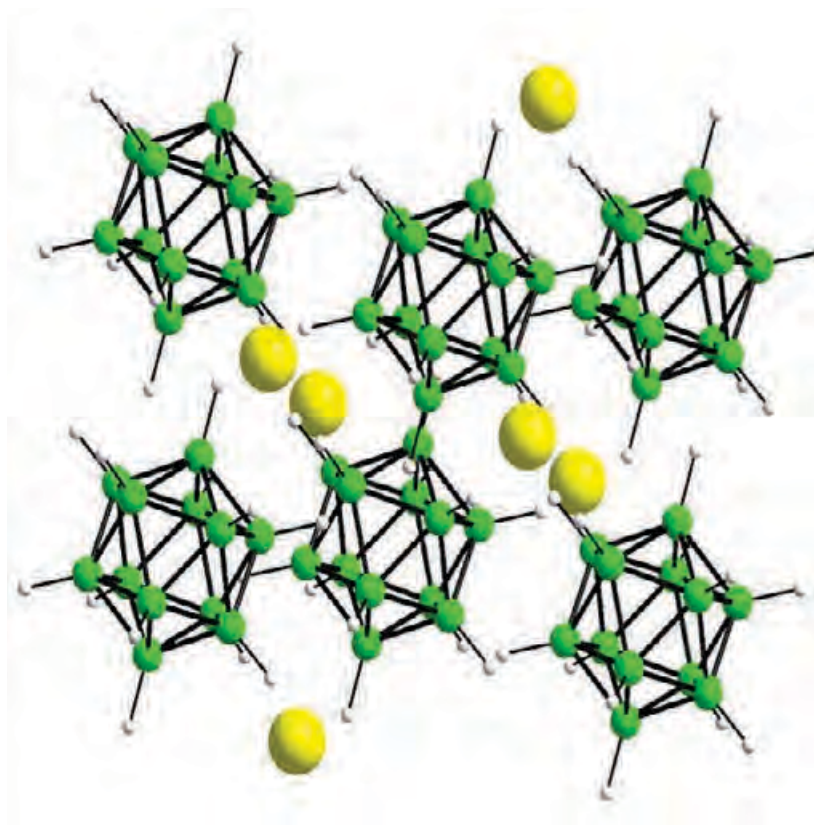
Structural features of metal dodecahydro-closo-dodecaborates

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Metal dodecahydro-closo-dodecaborates have been recently explored as materials for hydrogen storage and as promising ionic conductors. However, their utility as hydrogen storage media is impeded by their high thermal stability, kinetic limitations, and side reactions. The high thermal and chemical stability of these materials makes them interesting for solid battery membrane applications, however more work is needed to understand the complicated phase transitions which occur in many metal dodecahydro-closo-dodecaborates. Recent literature suggests that dodecahydro-closo-dodecaborate species are formed as stable intermediates during the dehydrogenation of metal borohydrides [1]. This hypothesis is especially intriguing in the context of high thermal stability reported for compounds containing icosahedral dodecahydro-closo-dodecaborate anions in the presence of hydrogen gas [2]. Here, a series of multi-component alkali, alkaline-earth and transition metal [B₁₂H₁₂]²⁻ compounds were isolated and characterized by single-crystal and powder X-ray diffraction techniques. Attempts to rehydrogenate M₂B₁₂H₁₂ and MB₁₂H₁₂ (where M= alkali or alkaline-earth metal) in the presence of the metal hydrides we made, and several compounds were found to be susceptible to dehydrogenation/rehydrogenation reactions. In addition, selected M₂B₁₂H₁₂ compounds were found to display high-temperature phases with increased values of alkali metal ionic conductivity.

[1] Hwang, S. J.; Bowman, R. C.; Reiter, et al., *J. Phys. Chem. C* 2008, 112, 3164-3169, [2] V. Stavila, J.-H. Her, W. Zhou, et al., *J. Solid State Chem.*, 2010, 183, 1133–1140



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