Abstract Submitted
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First-Principles Determination of Crystal Structures, Phase Stability, and Reaction Thermodynamics in the Li-Mg-Al-H Hydrogen Storage System[1] ALIREZA AKBARZADEH[2], California State University Northridge, CHRIS WOLVERTON[3], Northwestern University, VIDVUDS OZOLINS[4], University of California Los Angeles — First-principles DFT calculations have been used to investigate the crystal structures, thermodynamic stability, and decomposition pathways of Li-Mg-Al-H hydrogen storage compounds. We find that the recently discovered $LiMg(AlH_4)_3$ compound is marginally stable with respect to decomposition into $LiAlH_4$ and $Mg(AlH_4)_2$; however, we also find that $LiMg(AlH_4)_3$ is unstable with respect to H_2 release and decomposes exothermically into $LiMgAlH_6$, Al, and H_2 in excellent agreement with measurements. Using ICSD crystal structures database, we predict that the hypothetical $MgAlH_5$ compound should assume the orthorhombic $BaGaF_5$ prototype structure. We also discuss that phonon vibrations have sizeable effects on the enthalpies and entropies of hydrogen release reactions of Li-Mg-Al-H compounds.

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[2]Dept. of Physics & Astronomy
[3]Dept. of Materials Science and Engineering
[4]Dept. of Materials Science and Engineering

Alireza Akbarzadeh
California State University Northridge

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