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Phase Stability of Mixed-Alkali Alanates ZHU MA, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332, MEI-YIN CHOU, School of Physics, Georgia Institute of Technology, Atlanta, GA 30332 — To date sodium alanate NaAlH_4 is the only reversible complex hydride that satisfies the international density targets for hydrogen storage materials of 5 wt.% and 70 kg/m^3 . The reversible hydrogenation process takes place at reasonable conditions. Therefore, it is desirable to increase the H wt. partially replacing Na with a lighter alkali metal such as Li. To study the stability of these mixed-alkali alanates, we perform first-principles calculations for the alloy systems $\text{Na}_{1-x}\text{Li}_x\text{AlH}_4$ and $\text{Na}_{3(1-x)}\text{Li}_{3x}\text{AlH}_6$ within the framework of density functional theory and pseudopotentials. For the compositions we have considered for the tetrahydrides, the mixing energies are all positive, indicating that the sodium and lithium alanates prefer being phase separated. For the hexahydrides, one stable intermediate compound is found. The binding characteristics of these mixed-alkali alanates will be discussed.

Mei-Yin Chou
School of Physics, Georgia Institute of Technology, Atlanta, GA 30332

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