Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Theoretical study of the vibrational properties of $NaAlH_4$ with AlH_3 vacancies MEI-YIN CHOU, FENG ZHANG, YAN WANG, School of Physics, Georgia Institute of Technology — We investigate from first-principles calculations the vibrational properties in the presence of the AlH_3 vacancy in both α and γ phases of $NaAlH_4$. When AlH_3 is removed from an AlH_4^- anion, the remaining H recombines with another neighboring AlH_4^- anion and forms an AlH_5^{2-} unit with slightly deformed D_{3h} symmetry. For both α- and γ-$NaAlH_4$, the AlH_3 vacancy induces several isolated phonon modes that are highly localized on the AlH_5^{2-} unit with frequencies within the band gap separating the Al-H stretching modes and Al-H bending modes in pure $NaAlH_4$. Similar localized phonon modes also exist in the gap separating the Al-H bending modes and the modes involving the rotation of AlH_4^- anions for the γ phase. On the other hand, for both α and γ phases of $NaAlH_4$ with charged AlH_4^- vacancies, no isolated phonon modes were found to be localized in the vacancy region with frequencies within the band gap of the pure crystal. These theoretical findings suggest further experimental studies to identify the defects that are involved in the decomposition of $NaAlH_4$.

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Date submitted: 19 Nov 2010 Electronic form version 1.4