

Abstract Submitted  
for the MAR13 Meeting of  
The American Physical Society

**Neutron Scattering Studies of Destabilized Lithium Borohydride**

NINA VERDAL, NIST Center for Neutron Research; University of Maryland, TERENCE UDOVIC, NIST Center for Neutron Research, JOHN RUSH, NIST Center for Neutron Research; University of Maryland, ALEXANDER SKRIPOV, Institute of Metal Physics, Ural Division of the Russian Academy of Sciences — One of the most promising materials for hydrogen storage is lithium borohydride,  $\text{LiBH}_4$ , due to its high hydrogen mass fraction. However, applications require destabilization of the material in order to reduce the temperature and pressure required for hydrogen cycling. One possible avenue for destabilization has been via the use of mixed crystals, for example,  $\text{LiI}$  and  $\text{LiBH}_4$ , in which the relatively large iodide anion expands the crystal lattice of bulk  $\text{LiBH}_4$ . Here we present neutron scattering results comparing  $\text{BH}_4^-$  anion reorientational dynamics for bulk  $\text{LiBH}_4$  and the destabilized  $\text{LiI-LiBH}_4$  system. Quasielastic neutron scattering spectroscopy shows that at temperatures below room temperature, the reorientational dynamics for hexagonal  $\text{LiI-LiBH}_4$  is very similar to that of the high-temperature (380 K and above) hexagonal phase of  $\text{LiBH}_4$  instead of its low-temperature orthorhombic phase, which exhibits different dynamics. This is consistent with the behavior found using NMR spectroscopy.

Nina Verdal  
NIST Center for Neutron Research; University of Maryland

Date submitted: 07 Nov 2012

Electronic form version 1.4