Abstract Submitted
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Quasi-Elastic Neutron Scattering (QENS) Studies of Hydrogen Dynamics for Nano-Confined NaAlH4[1] TABBETHA DOBBINS, Rowan University, Dept. of Physics, SHATHABISH NARASEGOWDA[2], Louisiana Tech University, CRAIG BROWN, MADHUSUDAN TYAGI, TIMOTHY JENKINS[3], National Institute for Standards and Technology, Center for Neutron Research — The hydrogen dynamics of nano-confined sodium alanate (NaAlH4) has been studied using quasi-elastic neutron scattering (QENS). Results indicate thermodynamic destabilization is responsible for reduced desorption temperatures of NaAlH4 upon confinement within the nanopores of a metal organic framework (MOF). Both the bulk (microscale) NaAlH4 and the nanoconfined NaAlH4 data were fitted to re-orientation models which yielded corresponding percent mobile hydrogen and jump lengths. The jump lengths calculated from the nano-NaAlH4 were ≈2.5 Å, and in conformity with those jump lengths determined for bulk NaAlH4 of ≈2.3 Å. As much as 18 % of the hydrogen atoms were estimated to be mobile in the nano-NaAlH4 sample even at relatively low temperatures of 350 K. In contrast, bulk NaAlH4 shows less than 7 % mobile H-atoms even at higher temperatures of ≈450 K. The activation energy for the long range is 3.1meV.

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