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Determination of structure and phase transition of nanophase NH_3BH_3 embedded in MCM-41 mesoporous silica HYUNJEONG KIM, Los Alamos National Laboratory, ABHI KARKAMKAR, THOMAS AUTREY, Pacific Northwest National Laboratory, PETER CHUPAS, Argonne National Laboratory, THOMAS PROFFEN, Los Alamos National Laboratory — Nanocomposition of ammonia borane (AB), NH_3BH_3, by loading AB in a mesoporous silica has shown great improvement in the hydrogen storage properties [1]; faster hydrogen desorption was observed at reduced temperature and the formation of borazine, by-products that affects hydrogen purity, was significantly suppressed. Even though an improvement was striking, its lack of long-range structural order and relatively light composed elements hinder conventional structural analyses. We have employed the atomic pair distribution function (PDF) analysis to investigate the nanophase AB residing in mesoporous channels of MCM-41 [2]. Temperature dependent x-ray PDF study shows that the AB confined in pores does not undergo the orthorhombic to tetragonal phase transition at 225 K that was observed in the bulk molecular crystal. Instead, it stays in the high temperature tetragonal phase over a temperature range of 110-240 K and becomes amorphous above 240 K. [1] A. Gutowska *et al.*, *Angew. Chem. Int. Ed.*, **44**, 3578-3582 (2005). [2] H. J. Kim *et al.*, *J. Am. Chem. Soc.*, **131**, 13749-13755 (2009).

Hyunjeong Kim

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