

**NIST Center for Neutron Research
Hydrogen Storage Related Publications (2008)**

Metal Hydrides and Chemical Hydrides

1. J.-H. Her, M. Yousufuddin, W. Zhou, S.S. Jalilatgi, J.G. Kulleck, J.A. Zan, S.-J. Hwang, R.C. Bowman, Jr., and T.J. Udovic, "Crystal Structure of Li₂B₁₂H₁₂: a Possible Intermediate Species in the Decomposition of LiBH₄," *Inorg. Chem.* (in press).
2. H. Wu, W. Zhou, K. Wang, T.J. Udovic, J.J. Rush, T. Yildirim, L. Bendersky, A.F. Gross, and J.J. Vajo, "Size Effects on the Hydrogen Storage Properties of Nanoscaffolded Li₃BN₂H₈," *Nanotechnology* (in press).
3. H. Wu, "Strategies for the Improvement of the Hydrogen Storage Properties of Metal Hydride Materials," *ChemPhysChem* **9**, 2157 (2008).
4. H. Wu, W. Zhou, T.J. Udovic, J.J. Rush, and T. Yildirim, "Crystal Chemistry of Perovskite-type Hydride NaMgH₃: Applications for Hydrogen Storage," *Chem. Mater.* **20**, 2335 (2008).
5. H. Wu, "Structure of Ternary Imide Li₂Ca(NH)₂ and Hydrogen Storage Mechanisms in Amide-Hydride Systems," *J. Am. Chem. Soc.* **130**, 6515 (2008).
6. H. Wu, W. Zhou, and T. Yildirim, "Alkali and Alkaline-Earth Metal Amidoboranes: Structure, Crystal Chemistry, and Hydrogen Storage Properties", *J. Am. Chem. Soc.* (in press).
7. H. Wu, W. Zhou, T.J. Udovic, J.J. Rush, and T. Yildirim, "Structure and Crystal Chemistry of Isotopically-Labeled Li₂BNH₆ and Li₄BN₃H₁₀," *Chem. Mater.* **20**, 1245 (2008).
8. L. Senadheera, E.M. Carl, T.M. Ivancic, M.S. Conradi, R.C. Bowman, Jr., S.-J. Hwang, and T. J. Udovic, "Molecular H₂ Trapped in AlH₃ Solid," *J. Alloys Compd.* **463**, 1 (2008).
9. H. Wu, W. Zhou, T.J. Udovic, J.J. Rush, and T. Yildirim, "Structure Variations and Hydrogen Storage Properties of Ca₅Si₃ with Cr₅B₃-type Structure," *Chem. Phys. Lett.* **460**, 432 (2008).
10. J. Rijssenbeek, Y. Gao, J. Hanson, Q. Huang, C. Jones, B. Toby, "Crystal Structure Determination and Reaction Pathway of Amide-Hydride Mixtures," *J. Alloys Compd.* **454**, 233, (2008).
11. N.J. Hess, M.R. Hartman, C.M. Brown, E. Mamontov, A. Karkamkar, D.J. Hellebrant, L.L. Daemen, and T. Autrey, "Quasielastic Neutron Scattering of -NH₃ and -BH₃ Rotational Dynamics in Orthorhombic Ammonia Borane," *Chem. Phys. Lett.* **459**, 85 (2008).
12. R.O. Moyer Jr., M.A. Sytle, B.H. Toby, F.G. Morin, D.F.R. Gilson, "Neutron Powder Diffraction and Solid-State Deuterium NMR Studies of Ca₂RuD₆ and the Stability of Transition Metal Hexahydride Salts," *J. Alloys Compd.* **460**, 138 (2008).
13. M.M. Barsan, I.S. Butler, D.F.R. Gilson, R.O. Moyer, Jr., W. Zhou, H. Wu, and T.J. Udovic, "Raman, FTIR, Photoacoustic-FTIR, and Inelastic Neutron Scattering Spectra of Alkaline Earth and Lanthanide Salts of Hexahydroruthenate(II), A₂RuH₆, (A=Ca, Sr, Eu) and their Deuterides," *J. Phys. Chem. A* **112**, 6936 (2008).
14. T.J. Udovic, Q. Huang, A. Santoro, and J.J. Rush, "The Nature of Deuterium Arrangements in YD₃ and other Rare-Earth Trideuterides," *Z. Kristallogr.* (in press).
15. B. Hjörvarsson, G. Andersson, J.A. Dura, T.J. Udovic, P. Isberg, and C.F. Majkrzak, "Temperature Dependence of the Magnetic Interlayer Ordering in Fe(3)V(14)H_x (001) Superlattices," *Superlattices and Microstructures* **43**, 101 (2008).

Metal Organic Frameworks and other H₂ Physisorption Systems

16. Y. Liu, H. Kabbour, C.M. Brown, D.A. Neumann, and C.C. Ahn, "Increasing the Density of Adsorbed Hydrogen with Coordinatively Unsaturated Metal Centers in Metal-Organic Frameworks," *Langmuir* **24**, 4772 (2008).
17. Y. Liu, J.-H. Her, A. Dailly, A.J. Ramirez-Cuesta, D.A. Neumann, and C.M. Brown, "A Reversible Structure Transition of MIL-53 with Temperature Hysteresis," *J. Am. Chem. Soc.* **130**, 11813 (2008).
18. Y. Liu, C.M. Brown, D.A. Neumann, H. Kabbour, and C.C. Ahn, "Hydrogen Adsorption in MOF-74 Studied by Inelastic Neutron Scattering," in *Life Cycle Analysis for New Energy Conversion and Storage Systems*, edited by V.M. Fthenakis, A.C. Dillon, and N. Savage, Mater. Res. Soc. Symp. Proc. **1041**, R2_03 (2008).
19. C.M. Brown, Y. Liu, and D.A. Neumann, "Neutron Powder Diffraction of Metal-Organic Frameworks for Hydrogen Storage," *Pramana - J. Phys.* **71**, 755 (2008).
20. W. Zhou, H. Wu, and T. Yildirim, "Enhanced H₂ Adsorption in Isostructural Metal-Organic Frameworks with Open Metal Sites: Strong Dependence of the Binding Strength on Metal Ions," *J. Am. Chem. Soc.* (in press).
21. W. Zhou and T. Yildirim, "Nature and Tunability of Enhanced Hydrogen Binding in Metal-Organic Frameworks with Exposed Transition Metal Sites", *J. Phys. Chem. C* **112**, 8132 (2008).
22. S. Ma, D. Sun, J.M. Simmons, C.D. Collier, D. Yuan, H.-C. Zhou, "Metal-Organic Framework from an Anthracene Derivative Containing Nanoscopic Cages Exhibiting High Methane Uptake," *J. Am. Chem. Soc.* **130**, 1012 (2008).
23. J. Luo, H. Xu, Y. Liu, Y. Zhao, L.L. Daemen, C. Brown, T.V. Timofeeva, S. Ma, H.-C. Zhou, "Hydrogen Adsorption in a Highly Stable Porous Rare-Earth Metal-Organic Framework: Sorption Properties and Neutron Diffraction Studies," *J. Am. Chem. Soc.* **130**, 9626 (2008).
24. E. Durgun, S. Ciraci, and T. Yildirim, "Functionalization of Carbon-Based Nanostructures with Light Transition-Metal Atoms for Hydrogen Storage," *Phys. Rev. B* **77**, 085405 (2008).
25. Y. Yang, J. Schalch, Y. Liu, J.-H. Her, J. Simmons, C.M. Brown, P.A. Webley A.L. Chaffee, "Hydrogen Storage on Ordered Microporous Carbon Molecular Sieves Containing Dispersed Platinum Nanoparticles," *ACS Division of Fuel Chemistry Preprints* **53**, (2008).
26. X.-S. Wang, S. Ma, K. Rauch, J.M. Simmons, D. Yuan, X. Wang, T. Yildirim, W.C. Cole, J.J. López, A. de Meijere, H.-C. Zhou, "Metal-Organic Frameworks Based on Double-Bond-Coupled Di-Isophthalate Linkers with High Hydrogen and Methane Uptakes," *Chem. Mater.* **20**, 3145 (2008).
27. W. Zhou, H. Wu, T. Yildirim, J.R. Simpson, A.R. Hight Walker, "Origin of the Exceptional Negative Thermal Expansion in Metal Organic Framework-5 Zn₄O(1,4-benzenedicarboxylate)₃," *Phys. Rev. B* **78**, 054114 (2008).
28. W. Zhou, H. Wu, T.J. Udovic, J.J. Rush, and T. Yildirim, "Quasi-free Methyl Rotation in Zeolitic Imidazolate Framework-8," *J. Phys. Chem. A* (in press).