

MAR09-2008-000492

Abstract for an Invited Paper
for the MAR09 Meeting of
the American Physical Society

Computational methods to determine the structure of hydrogen storage materials¹

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To understand the mechanisms and thermodynamics of material-based hydrogen storage, it is important to know the structure of the material and the positions of the hydrogen atoms within the material. Because hydrogen can be difficult to resolve experimentally computational research has proven to be a valuable tool to address these problems. We discuss different computational methods for identifying the structure of hydrogen materials and the positions of hydrogen atoms, and we illustrate the methods with specific examples. Through the use of ab-initio molecular dynamics, we identify molecular hydrogen binding sites in the metal-organic framework commonly known as MOF-5 [1]. We present a method to identify the positions of atomic hydrogen in imide structures using a novel type of effective Hamiltonian. We apply this new method to lithium imide (Li_2NH), a potentially important hydrogen storage material, and demonstrate that it predicts a new ground state structure [2]. We also present the results of a recent computational study of the room-temperature structure of lithium imide in which we suggest a new structure that reconciles the differences between previous experimental and theoretical studies.

[1] T. Mueller and G. Ceder, Journal of Physical Chemistry B 109, 17974 (2005).

[2] T. Mueller and G. Ceder, Physical Review B 74 (2006).

¹Supported by the U.S. Department of Energy grant DE-FG02-05ER46253.