Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Charge-Driven Structural Transformation and Valence Versatility of Boron Sheets in Magnesium Borides[1] YUFENG ZHAO, National Renewable Energy Laboratory, CHUNMEI BAN, QIANG XU, SUHUAI WEI, ANNE C. DILLON, NATIONAL RENEWABLE ENERGY LABORATORY TEAM — We show here that boron sheets exhibit highly versatile valence and the layered boron materials may hold the promise for a high energy-density magnesium-ion battery. Practically, boron is superior to previously known multi-valence materials, especially transition metal compounds, which are heavy, expensive, and often not benign. Based on Density Functional Theory simulations, we have predicted a series of stable magnesium borides MgBx with a broad range of stoichiometries, $2 < x \leq 16$, by removing magnesium atoms from MgB2. The layered boron structures are preserved through an in-plane topological transformation between the hexagonal lattice domains and triangular domains. The process can be reversibly switched as the charge transfer changes with Mg insertion/extraction. The mechanism of such a charge-driven transformation originates from the versatile valence state of boron in its planar form. The discovery of these new physical phenomena suggests the design of a high-capacity magnesium-boron battery.

[1]Funded by the U.S. Department of Energy under subcontract number DE-AC36-08GO28308 through: DOE Office of Energy Efficiency and Renewable Energy Office of the Vehicle Technologies Program.

Yufeng Zhao
National Renewable Energy Laboratory

Date submitted: 18 Nov 2010 Electronic form version 1.4