NREL Highlights SCIENCE

Density Functional Theory Simulations Predict New Materials for Magnesium–Ion Batteries

Multivalence is identified in the light element, B, through structure morphology.

Boron sheets exhibit highly versatile valence, and the layered boron materials may hold the promise of a high-energy-density magnesium-ion battery. Practically, boron is superior to previously known multivalence materials, especially transition metal compounds, which are heavy, expensive, and often not benign.

Based on density functional theory simulations, researchers at the National Renewable Energy Laboratory (NREL) have predicted a series of stable magnesium borides, MgB_x, with a broad range of stoichiometries, $2 < x < 16$, by removing magnesium atoms from MgB_2. The layered boron structures are preserved through an in-plane topological transformation between the hexagonal lattice domains and the 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 with theoretical energy density 876 mAh/g and 1550 Wh/L.

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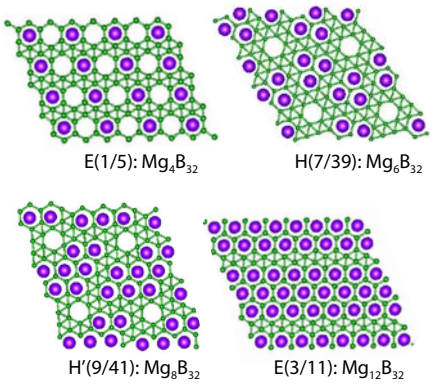
Reference: Zhao, Y.; Ban, C.; Xu, Q.; Wei, S–H.; Dillon, A. "Charge-Driven Structural Transformation and Valence Versatility of Boron Sheets in Magnesium Borides." *Phys. Rev. B* **83**, 035406 (2011).



Atomic structures (projected in the x-y plane) of four magnesium borides derived from MgB_2 through the reaction $Mg_{16}B_{32} \rightleftharpoons Mg_NB_{32} + (16 - N)$ Mg. The boron sheets are shown by web-like balls and sticks. The bigger balls (purple) denote Mg ions intercalated between the boron layers in the z direction. Four super cells are plotted for each case.

Key Research Results

Achievement

Based on density functional theory simulations, NREL researchers have predicted a series of stable magnesium borides with a broad range of stoichiometries by removing magnesium atoms from MgB_2.

Key Result

These structures exhibit highly versatile valence, and boron is superior to previously known multivalence materials, especially transition metal compounds, which are heavy, expensive, and often not benign.

Potential Impact

The discovery of these new physical phenomena suggests the design of a high-capacity magnesium-boron battery.

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