

Supporting Information

Lithium-ion Battery Electrode Properties of Hydrogen Boride

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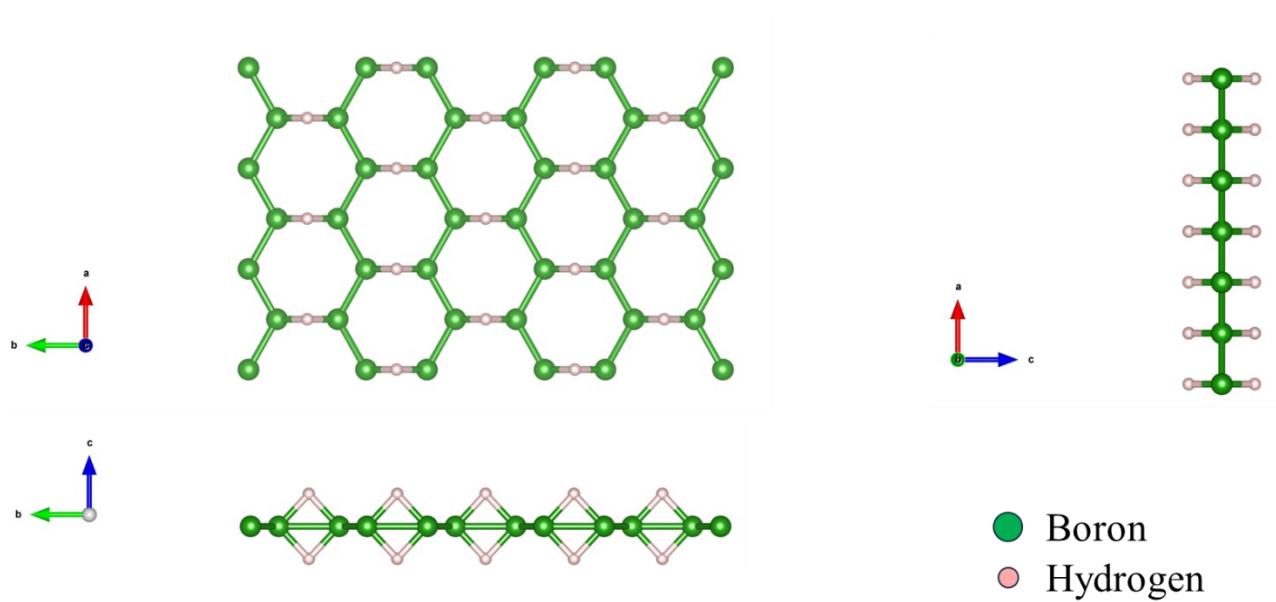


Fig. S1 The expected atomic structure of the HB sheet.

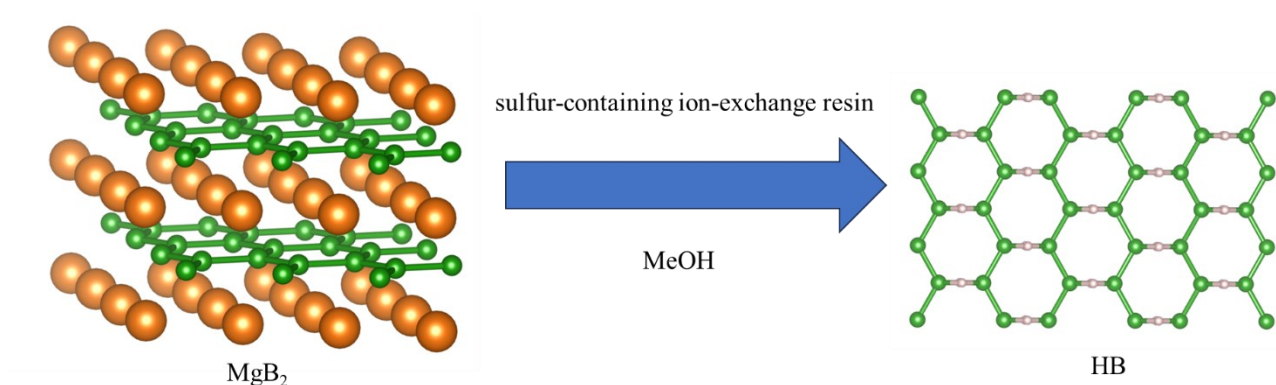


Fig. S2 The synthesis procedure of HB.

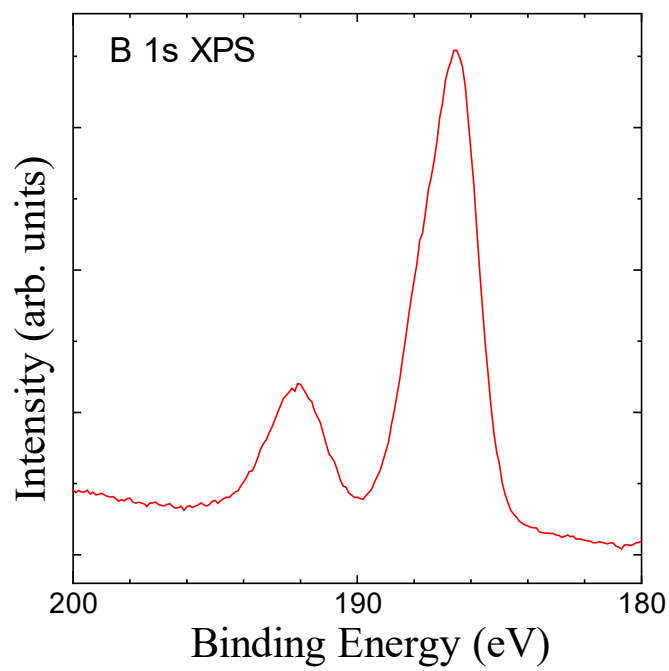


Fig. S3 B 1s XPS spectrum of the partially oxidized HB.

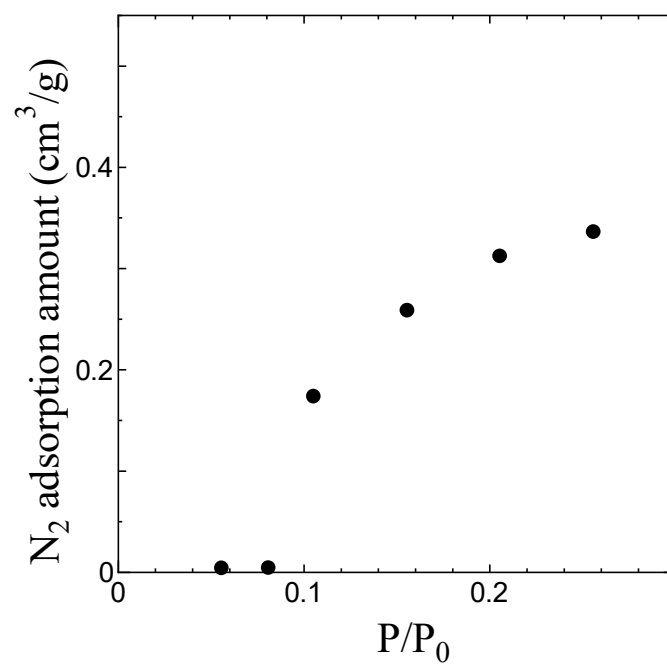


Fig. S4 N_2 gas adsorption isotherm of the prepared HB sample. Blank correction treatment was not applied.

Calculation of specific surface area of HB

Here, we calculate the area of the hexagonal lattice of boron (Fig. S1) and determine the specific surface area by dividing it by the molecular weight of HB (11.819). The area associated with the B-H-B in Fig. S1 is disregarded.

According to literature, the B-B bond lengths are known to be 1.81 and 1.72 Å. Therefore, the area can be calculated from simple geometry as shown in the figure. Since this hexagon contains two molecules of HB, the specific surface area is obtained by dividing the previously calculated area by the mass of two HB molecules.

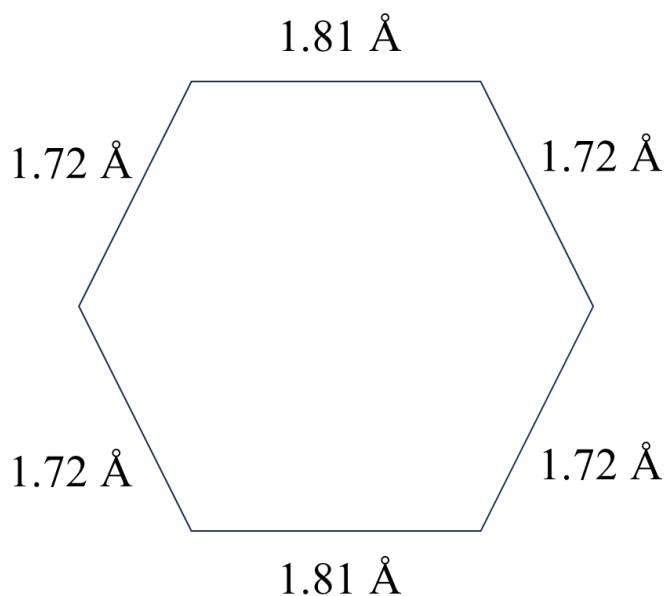


Fig. S5 B-B bond lengths of boron quasi-hexagon ring in HB.

Calculating under the aforementioned assumptions, we obtain a specific surface area of 4049 m²/g for HB.

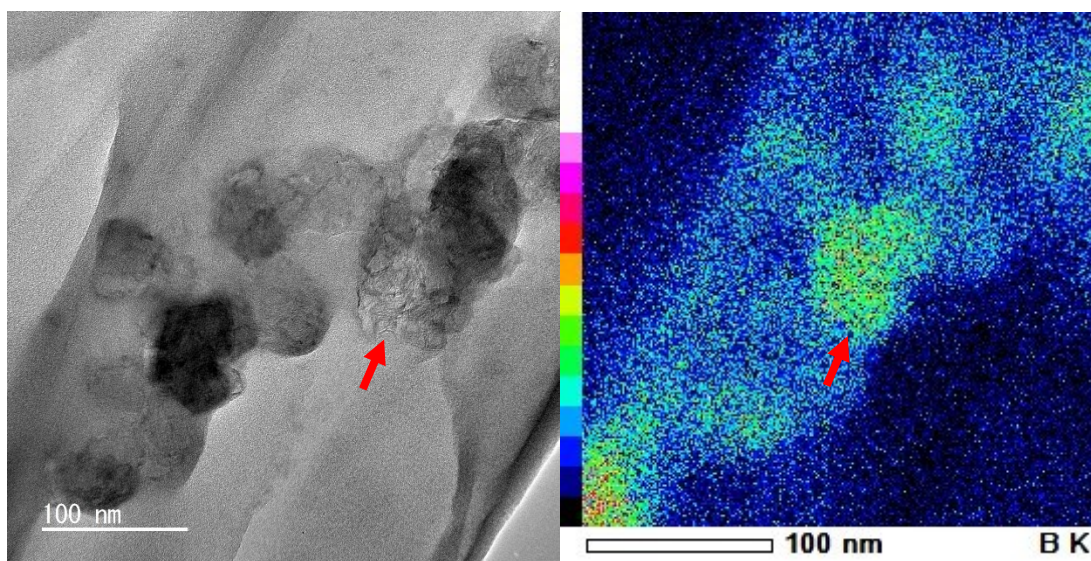


Fig. S6 TEM image and corresponding B EDS mapping image of the battery electrode sample including HB after the charge-discharge experiments. The section pointed to by the arrow is considered to be the HB sample.

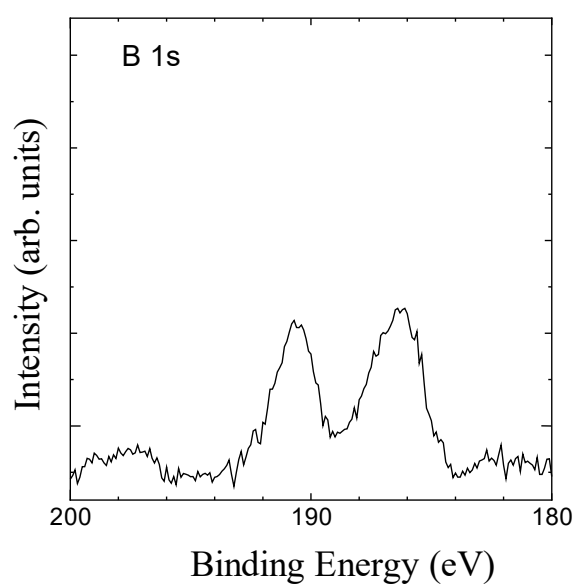


Fig. S7 B 1s XPS spectrum of the battery electrode sample including HB after the charge-discharge experiments.