Earth-abundant iron diboride (FeB2) nanoparticles as highly active bifunctional electrocatalysts for overall water splitting

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Abstract:

Developing efficient, durable, and earth-abundant electrocatalysts for both hydrogen and oxygen evolution reactions is important for realizing large-scale water splitting. We report that FeB_2 nanoparticles, prepared by a facile chemical reduction of Fe^{2+} using $LiBH_4$ in an organic solvent, are a superb bifunctional electrocatalyst for overall water splitting. The FeB_2 electrode delivers a current density of 10 mA/cm^2 at overpotentials of 61 mV for hydrogen evolution reaction (HER) and 296 mV for oxygen evolution reaction (OER) in alkaline electrolyte with Tafel slopes of 87.5 and 52.4 mV/dec, respectively. The electrode can sustain the HER at an overpotential of 100 mV for 24 h and OER for 1000 cyclic voltammetry cycles with negligible degradation.

DFT calculations demonstrate that the boron-rich surface possesses appropriate binding energy for chemisorption and desorption of hydrogen-containing intermediates, thus favoring the HER process. The excellent OER activity of FeB_2 is ascribed to the formation of FeOOH/FeB_2 heterojunction during water oxidation. An alkaline electrolyzer is constructed using two identical FeB_2-NF electrodes as both anode and cathode, which can achieve a current density of 10 mA/cm^2 at 1.57 V for overall water splitting with faradaic efficiency of nearly 100 %, rivalling the integrated state-of-the-art Pt/C and RuO_2/C.

Contribution: Invited