# $AlFe_2B_2$: Electrocatalytic Water Oxidation with Earth-Abundant Elements

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## Background and Significance

The depletion of fossil fuels worldwide and increased desire for clean-energy has driven research aimed at developing renewable energy sources[1]. Water electrolysis, the splitting of water molecules through hydrogen evolution reactions (HER) and oxygen evolution reactions (OER) (Fig. 1), is thought to be a possible clean energy source[2].

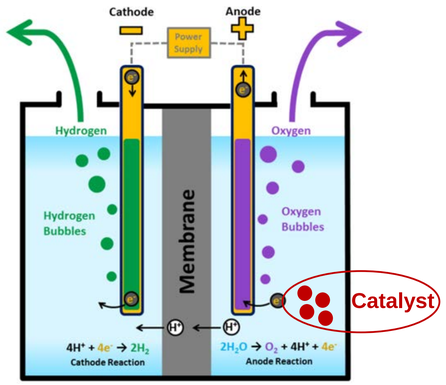



**Fig. 1** HER & OER reactions with catalyst

**At this time, the amount of energy required by water electrolysis is larger than the minimum thermodynamic value of 1.23 V, making it an ineffective substitute for fossil fuels.**

To reduce the thermodynamic value of these reactions, scientists are researching earth-abundant metals that will act as catalysts, to drive down the amount of energy required.

Investigation has identified that the layered crystal structure of $AlFe_2B_2$ (Fig. 2) affords efficient oxygen evolution reactions (OER) with a low over potential and high stability of the electrocatalyst[1].

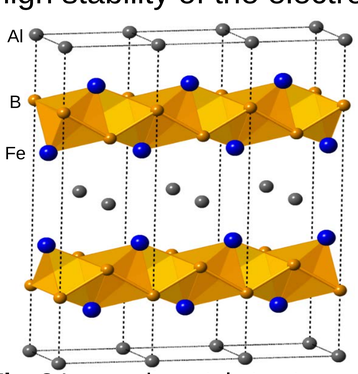



**Fig. 2** Layered crystal structure of $AlFe_2B_2$

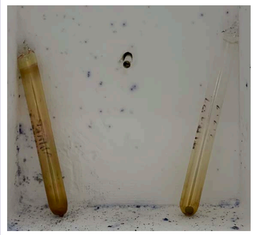
**To further increase the efficiency of the $AlFe_2B_2$ complex in OER reactions, what is the most economical synthesis method for making $AlFe_2B_2$ in a commercial setting?**

## Materials

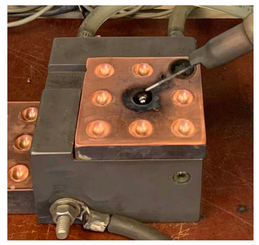
**Materials:** Aluminum powder (99.95%) and boron powder (95–97%) were used as received. Iron powder (98%) was further purified by heating in a flow of $H_2$ gas at 500 ˚C for 5 hours.

**Sample preparation:** All operations were carried out in an argon-filled glove box (concentration of oxygen < 1 ppm at.0.0 - 0.2). The metals were mixed in 3:2:2 ratio (unless otherwise noted) and pressed into a 10mm pellet, and then removed for synthesizing.

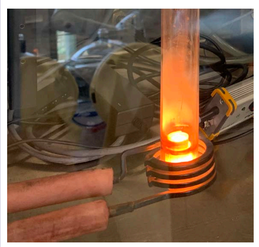
## Synthesis Techniques



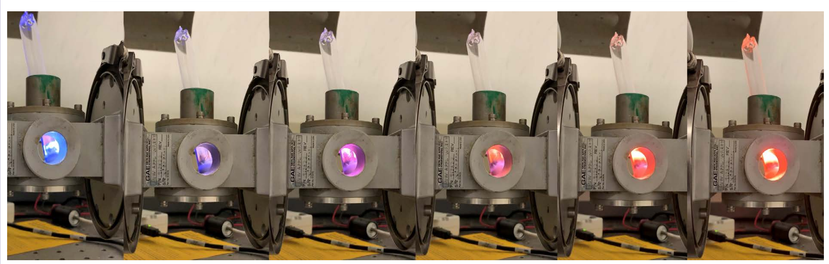
**Annealing:** Samples were sealed in a silica tube under vacuum (~$10^{-5}$ Torr) and heated in a furnace at 900 ˚C for 7 days.



**Arc-melting:** Samples were subjected to an electric arc struck between a tungsten electrode and the pellet, which was placed in a copper hearth and then annealed for 7 days.



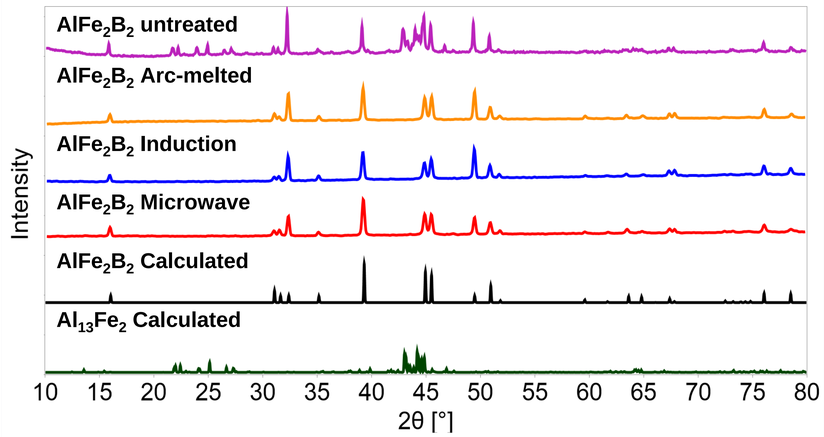
**Induction Heating:** Samples (stoichiometry 7:7:6) were placed in three sets of crucibles and positioned within a coil system. Alternating currents were used to heat samples to 1600 ˚C over 1 hour.



**Microwave:** Samples (stoichiometry 3:2.55:2) were placed in ceramic crucible insulated with glass wool and sealed in a silica tube. The samples were then subjected to 0.5 kW microwave power for 5 minutes.

## Powder X-ray Diffraction (PXRD)

After samples were homogenized through synthesis, the material was finely ground and mounted onto a PXRD plate. To further purify the sample, it was treated with diluted (1:1 v/v) HCl aqueous solution and PXRD was repeated. All results are provided for comparison.




## Conclusion

Synthesis of the layered crystal structure of $AlFe_2B_2$ can be accomplished through a number of techniques. These techniques can be used to further explore the use of $AlFe_2B_2$ and other earth-abundant elements as electrocatalysts for water electrolysis. Microwave synthesis is shown to be the most time efficient and effective method for synthesizing catalysts.

## References

1. Mann, D. K., et al. *Chem. Sci.*, **2019**, *10*, 2796
2. McCrory, C. C. L., et al. *J. Am. Chem. Soc.* **2015**, 137, 4347

## Acknowledgements

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