VIDEO ARTICLE

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Designing Boride Electrocatalysts for Hydrogen Evolution

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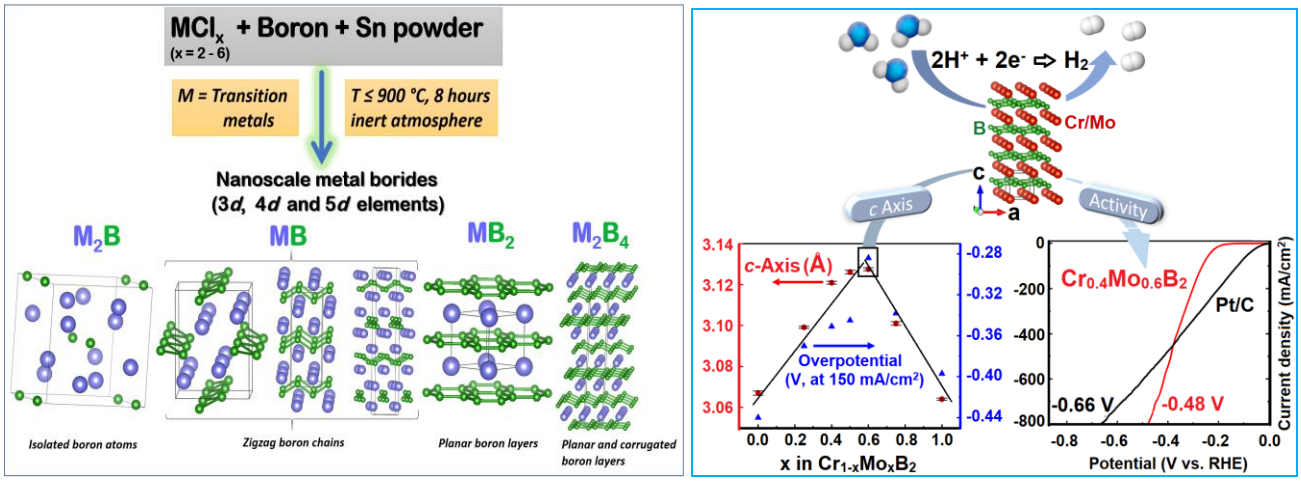
Graphical Abstract



Abstract

The electrolysis of water is considered as a clean mean for large scale hydrogen gas production. However, this large-scale production is still hindered by the high cost and scarcity of noble metal catalysts such as Pt. Recently, non-noble metal materials have emerged as highly active electrocatalysts (AlB_2-type) for the hydrogen evolution reaction (HER) to produce hydrogen. Our recent research found that α-MoB_2 [**1**] exhibits high HER activity. In addition, density functional theory (DFT) calculations show that several surfaces of MoB_2 are active and the optimum evolution of H_2 occurs on the graphene-like B-terminated {001} surface. Furthermore, DFT and experiments demonstrate that α-MoB_2 is more HER active than α-MoB_2 [**2**], due to the presence of 50% more graphene-like boron layers in the former It was recently also found that FeB_2 is highly active for

overall water splitting in basic solution. However, TiB_2 is not as active as MoB_2 for HER. To examine the distinct activities of metal diboride as HER electrocatalysts and how the metals could affect the graphene-like boron layer, DFT was applied to investigate the H-surface adsorption process on MB_2 (M = Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W). Our results indicate that the H-surface binding energy decreases as the electronegativity of the metal increases. Therefore, the electron transfer between metal and boron is one of the key parameters to control the HER activity of MB_2. Using a recently developed synthesis, [**3**] we were able to synthesize most of the above-mentioned diborides at the nanoscale. VB_2 behaves similarly to MoB_2, thus it was predicted by DFT to be a highly active HER catalyst candidate and confirmed by experiments. Subsequently, an unexpected boron-chain dependency of the HER activity was discovered in vanadium borides, that enabled not only the prediction of the HER activity of unstudied V_2B_3 but also those of other hypothetical "V_xB_y" were predicted using an exponential equation that predicts the overpotentials of known and hypothetical V_xB_y phases containing at least a boron chain. [**4**] We have also recently discovered an unexpected lattice parameter-dependency on HER of ternary variants with the AlB_2-type structure that has enabled an excellent boride HER electrocatalyst that outperforms Pt/C at high current density. [**5**]

Keywords: Hydrogen evolution; borides; electrocatalysis; AlB_2-type; current density.

Acknowledgements

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References

1. H. Park, et al., *Angew. Chem. Int. Ed.* **2017**, 56, 5575.
2. H. Park, et al., *J.Amer.Chem.Soc.* **2017**, 139, 12915.
3. P. R. Jothi, et al., *Adv. Mater.* **2018**, 30, 1704181.
4. E. Lee, et al., *Angew. Chem. Int. Ed.* **2020**, https://doi.org/10.1002/anie.202000154.
5. H. Park, et al., *Adv. Mater.* **2020**, accepted.

Biography of Presenting Author

Boniface P. T. Fokwa obtained his BS and MS from University of Yaounde I (Cameroon), his PhD from Dresden University of Technology (Germany) in 2003 and his Habilitation from RWTH Aachen University (Germany) in 2010. After working for four and half years as Heisenberg Fellow at RWTH he accepted an Assistant Professor position at University of California Riverside in 2015 and was promoted to Associate Professor with tenure in 2018. He is a recipient of several awards including a DFG postdoctoral fellowship (2004-2006), a Heisenberg Fellow Award (2011-2015, from the German research foundation, DFG) and an NSF CAREER Award (2017-2021). He was a visiting scientist at the University of Auckland (New Zealand, 2011), at Cornell University (USA, 2012) and a visiting Professor at the University of California, Los Angeles (USA, 2014-2015). He serves as Section Editor for Encyclopedia of Inorganic and Bioinorganic Chemistry. His research group combines experimental and computational methods to rationally design materials for

energy-related applications such as magnets, superconductors, and catalysts. He has co-authored a book, a book chapter and 115 peer-reviewed publications so far.

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