2nd October 2025
13:30-14:30
総合研究棟 B310

Designing Earth-Abundant Bulk and Nano-Electrocatalysts for Hydrogen Production

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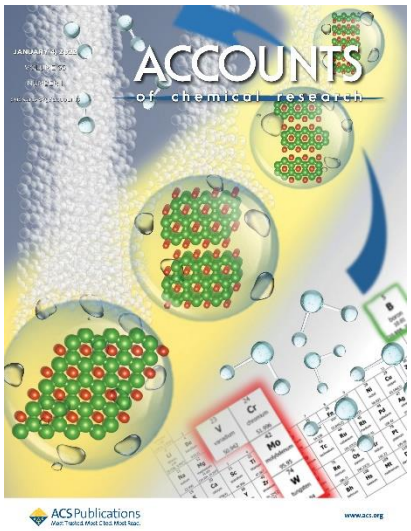
The electrolysis of water is considered as a clean means for large scale hydrogen gas production. [1] However, this large-scale production is still hindered by the high cost and scarcity of noble metal catalysts such as Pt. Recently, non-noble metal materials have emerged as highly active electrocatalysts for the hydrogen evolution reaction (HER) to produce hydrogen. Our recent research found that α-MoB_2 (AlB_2-type, a 2D-like structure) exhibits high HER activity. [2] In addition, density functional theory (DFT) calculations show that several surfaces of α-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 β-MoB_2 [3], 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. [4] To examine the distinct activities of metal diboride as HER electrocatalysts and demonstrate how different transition 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, [5] 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 (Figure below). [6] We have also recently found an unexpected lattice parameter-dependency on HER of ternary variants crystallizing with the AlB_2-type structure that allowed $Cr_{0.4}Mo_{0.6}B_2$ to overpower Pt/C at high current density. [7] Furthermore, an unexpected boron-chain dependency of the HER activity was discovered in the V-B system, [8] that even allows for the prediction of unknow active HER catalysts. These results have recently been summarized in an invited account. [9]



References
(1) Seh et al., *Science*, 355, eaad4998, (2017).
(2) H. Park, et al., *Angew. Chem. Int. Ed.* 56, 5575 (2017).
(3) H. Park, et al., *J. Amer. Chem. Soc.* 139, 12915 (2017).
(4) H. Li et al., *Adv. Energy Mater.* 7, 1700513 (2017).
(5) P. R. Jothi, et al., *Adv. Mater.* 30, 1704181 (2018).
(6) P. R. Jothi, et al., *ACS Appl. Energy Mater.* 30, 1704181 (2018).
(7) H. Park, et al., *Adv. Mater.* 32, 2000855 (2020).
(8) E. Lee, et al., *Angew. Chem. Int. Ed.* 59, 11774 (2020).
(9) E. Lee, B.P.T. Fokwa, *Acc. Chem. Res.* 55, 56 (2022).

Biography:

Professor of Chemistry	since **2021**
Associate Professor of Chemistry	**2018-2021**
Chair, ACS Solid State Chemistry Subdivision	**2022**
Section Editor for EIBC	since **2018**
Assistant Professor of Chemistry	**2015-2018**
NSF CAREER Award	**2016**
Associate Editor for EIBC	**2016-2018**
Visiting Professor, UC Los Angeles, USA	**2014-2015**
Heisenberg Fellow, German Research Foundation	**2011-2014**
Visiting scientist, Cornel University, Ithaca,USA	**2012**
Visiting scientist, Univ. of Auckland, New Zealand	**2011**
Postdoctoral Fellow, German Research Foundation	**2004-2006**
Ph.D (Dr.rer.nat.): Dresden University of Technology	**2003**
BS, MS: University of Yaounde I(Cameroon)	**1996, 1998**