Computational study of pentlandites for the oxygen evolution reaction

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ABSTRACT

There is an ever-growing interest in green hydrogen, which is produced by electrolytic water splitting. The efficiency of green hydrogen production is limited by the sluggish four-electron oxygen evolution reaction (OER). This process is facilitated by selecting an efficient catalyst as the anode material, and there is an ongoing search for efficient and sustainable electrocatalysts.

Pentlandites, $(Fe_xNi_{9-x})S_8$ (cf. Figure 1), are a promising class of materials for water splitting [1] consisting of earth-abundant elements. They are easy to synthesize and exhibit high catalytic activity for the alkaline OER. Despite the experimental evidence for the use of pentlandites as an OER catalyst, a detailed investigation of the elementary reaction steps, including consideration of adsorbate coverages and limiting steps under anodic polarizing conditions, is still missing. We address this gap by gaining atomistic insights into the OER on a $Fe_{4.5}Ni_{4.5}S_8(111)$ surface through density functional theory calculations combined with descriptor-based analysis. This allows us to present general guidelines for modeling OER on complex material compositions. [2]

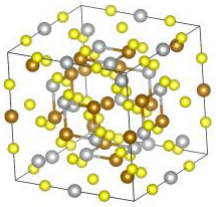

Figure 1. Bulk structure of $Fe_{4.5}Ni_{4.5}S_8$.

References

[1] H. M. A. Amin, M. Attia, D. Tetzlaff, U. Apfel Tailoring the Electrocatalytic Activity of Pentlandite Fe x Ni 9-X S 8 Nanoparticles via Variation of the Fe : Ni Ratio for Enhanced Water Oxidation. *ChemElectroChem* **2021**, *8*, 3863–3874.

[2] M. Sokolov and K. S. Exner, *Phys Chem Chem Phys* **2024**, submitted.