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M2 Internship

Mechanistic Study of the Hydrogen Evolution Reaction Over VS_2 via Atomistic Modelling

Context

The theoretical chemistry group of the Laboratoire de Chimie (LCH) at the ENS de Lyon has a strong expertise in modelling heterogeneous electrocatalysis. In collaboration with experiments carried out at the East China Normal University (ECNU) by Chaolun Wang, we will explore the properties of VS_2 under water-splitting conditions.

Background

The efficient production of hydrogen from renewable feedstocks is a key challenge. While water electrolysis is, in principle, a green process, electrocatalysts are necessary to achieve water splitting at near optimum electrochemical potentials. For the hydrogen evolution reaction (HER) in acidic conditions noble metals (e.g., platinum) constitute the state-of-the-art catalysts. These metals are too rare and expensive to envision their large-scale utilization for water electrolysis. Therefore, the development of stable and active electrocatalysts based on earth abundant elements is the goal of our project. Catalysts based on dichalcogenides are particularly promising, given their relatively high activity, stability and earth abundance. [Benck et al., ACS Catal. 2014, 4, 3957-3971] An on-going collaboration between LCH and IFP Energies Nouvelles is devoted to the mechanistic investigation of HER on MoS_2 [Abidi et al. ACS Appl. Mater. Interfaces, 2020, 12, 31401]. An interesting alternative in the same family are vanadium based catalysts[Wang et al, Applied Physics Letters, 2019, 114, 023902].

Project

Computational modelling is ideally suited to study the surface state (and thus the morphology), stability and HER activity of electrocatalysts. In combination with advanced surface characterizations, such as in-situ transmission electrical microscope (TEM) carried out at ECNU, this computational study will investigate the properties of VS_2 as an electrocatlyst. LCH has ample experience in modelling electrocatalysis under realistic conditions, and in particular including the effect of the electrochemical potential and the electrolyte. [Abidi et al. WIREs Comput Mol Sci. 2021; 11, e1499].

This internship will be carried out under the co-supervision of Nawras Abidi who is currently working on HER on MoS_2.

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