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PhD Fellowship

Characterization of the Active Sites of MoS_2 in Electrocatalysis via Atomistic Modelling

Context

The theoretical chemistry group of the Laboratoire de Chimie at the ENS de Lyon has a strong expertise in modelling heterogeneous catalysis. The project MoSHy, funded by the region Rhône-Alpes-Auvergne, is carried out in strong collaboration with the IFP Energies nouvelles (Solaize).

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) 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 (in particular MoS_2), given their relatively high activity, stability and earth abundance. [Benck et al., ACS Catal. 2014, 4, 3957-3971]

Project

Within this project, we will exploit the internationally recognized expertise of IFPEN (Solaize) in producing MoS_2 based catalysts, in combination with advanced, atomistic, computational modelling at the laboratory of Chemistry at ENSL. The project furthermore will benefit from the unique characterization capabilities of the LEPMI (Grenoble) under electrochemical conditions.

Computational modelling is ideally suited to study the active sites, stability and conductivity as a function of the microstructure of the catalyst. In particular, the surface state and the influence of doping can be assessed as a function of the electrochemical potential and pH. This study, in combination with advanced surface characterizations to validate the computational results allows to propose the most promising active sites and thus direct the synthesis towards a maximization of these sites. Indeed, the team of ENSL has recently gained experience in modelling electrocatalysis under ever more realistic conditions, including the effect of the electrochemical potential and the electrolyte. [Steinmann, Sautet, J. Phys. Chem. C 2016, 120, 5619].

Depending on the candidate, parts of the experimental surface characterizations might be carried out by the PhD student or by Master students hired separately.

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