Kolloquium des Wilhelm-Ostwald-Instituts

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Theoretical Description of Energy Storage and Conversion Processes

Abstract

Electrochemical processes for energy storage or conversion require efficient electrocatalysts to enhance intrinsic activity as well as to minimize energy losses in terms of applied overpotential. Since the initial works of Nørskov and coworkers, it is believed that the understanding of correlations between materials in a homologous series contributes to the rational design of electrocatalysts [1]. In this context, volcano plots have been largely used to capture the trends of electrocatalytic processes, thereby relying on scaling relations and thermodynamic considerations at the equilibrium potential by connecting the thermodynamics to the kinetics via the Sabatier principle and Brønsted−Evans−Polanyi (BEP) relation [2]. In the first part of my lecture, I am going to highlight recent advances relating to the construction of volcano plots by the descriptor $G_{max}(\eta)$, a potential-dependent activity measure based on the notion of the free-energy span model [3]. Notably, the impact of the volcano slope and various mechanistic pathways for volcano analyses is stressed [4], demonstrating that
a) the volcano slope is prone to change at the leg of the volcano plot [5];
b) the consideration of traditional mechanisms only is insufficient for proper description of highly active catalysts [6].

In the second part of my lecture, I discuss recent advances in the realm of single-atom catalysts (SACs) for chlorine evolution (CER), an important electrochemical half-cell reaction for chemical industry to produce gaseous chlorine [7]. Applying a combined experiment-theory approach, we demonstrated the importance of various active sites to comprehend the high activity and stability of Pt-based SACs in the CER [8].

References:
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