Modeling protocols for ORR and OER catalysts in solar water splitting

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A limiting factor in solar water splitting are the catalysts for the oxygen reduction reactions (ORR) and oxygen evolution reactions (OER). The state-of-the art catalysts for these reactions, Pt and Ir, are precious metals which contribute to the high capital cost and do not provide a sustainable solution to this problem. Recently discovered transition-metal derived nitrogen doped graphene (TMDNGs) catalysts have shown comparable activity to Pt and Ir in alkaline media. However, performance still lags behind in acidic environment. The search for next-generation catalyst systems is thus crucial to move this technology forward.

Our research concerns the development of accurate and robust computational protocols to model the solvent-catalyst interactions during the ORR and OER reactions in TMDNGs. Various models are benchmarked and evaluated on a cost vs. accuracy trade-off. Our results are compared with similar studies on other photo-catalytic systems, e.g., CoP_is (Cobalt-phosphate based systems mimicking an 'artificial leaf'). The best model will then be applied to in a virtual high-throughput investigation of thousands of catalyst candidates, which will subsequently lead to the identification of key descriptors for catalyst performance for both the OER and ORR. The obtained structure-property relationships will serve as the foundation for rational design efforts towards highly efficient non-precious metal catalysts.