Carbon-Based 2D Electrocatalysts for Efficient Water Splitting

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Abstract

One of the technological routes for achieving net-zero emissions is the use of low carbon hydrogen, for which more efficient and cheaper production technologies are needed. Two-dimensional (2D) carbon-based materials, including graphene and its doped variants, have gained significant attention as viable alternatives to noble metals for electrochemical water splitting due to their abundance, stability, and tunable electronic properties. Studies indicate that heteroatom-doped graphene and 2D porous carbon nanosheets demonstrate promising performance for water splitting; hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) [1], [2]. Specifically, nitrogen and sulfur doping in graphene improves electron density distribution, creating active sites favorable for catalytic activity, especially under alkaline conditions [3]. Doped carbon structures additionally exhibit enhanced durability and efficient mass transport due to minimized catalyst aggregation [4]. Dual-doped graphene, for instance, has shown competitive catalytic performance with reduced overpotentials and enhanced kinetics in both HER and OER processes [5]. The objective of this work is to explore the potential of noble metal-free carbon-based electrocatalysts as cost-effective options for sustainable hydrogen production by a combined computational modeling – experimental approach. Density Functional Theory (DFT) calculations are used to study and optimize selected novel 2D materials, aiming to identify electrocatalysts with improved performance for scalable green hydrogen production.
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References

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