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Evaluation of doped graphene materials for electrochemical hydrogen evolution reaction and oxygen reduction reaction

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The dwindling supply of fossil fuels urges us to explore alternative power sources to drive our highly automotive society. Under this background, establish reliable clean and sustainable energy supplies are of great importance, and using electrochemical method to realize energy conversions hold a great promise. Among these reactions, hydrogen evolution reaction (HER) and oxygen reduction reaction (ORR) are the most studied, due to their fundamentality in electrocatalysis and their role in hydrogen production and fuel cells, respectively. Effective candidates for these two reactions are often based on noble metals, while carbon-based metal-free electrocatalysts generally demonstrate poorer activity. Here we report evaluation of a series of heteroatom-doped graphene materials as efficient HER and ORR electrocatalysts by density functional theory calculations, with the input of spectroscopic characterizations and electrochemical measurements. Results of theoretical computations are shown to be in good agreement with experimental observations regarding the intrinsic electrocatalytic activity and the reaction mechanisms for these two reactions. As a result, we establish volcano shaped activity trends for HER and ORR on graphene-based materials, and explore their reactivity origin to guide the design of more efficient electrocatalysts. We predict that by rationally modifying particular experimentally achievable physicochemical characteristics, a practically realizable graphene-based material will have the potential to exceed the performance of the metal-based benchmarks for these two reactions.

Biography

Yan Jiao has her research interests in discovering the origin of electrocatalytic activity possessed by carbon-based materials by computational chemistry. She also aims to design novel carbon-based catalysts for clean energy conversion reactions, including hydrogen evolution reaction, oxygen reduction reaction and carbon dioxide reduction reaction. She obtained her PhD in Chemical Engineering from the University of Queensland, and is currently working as a Post-doctoral Researcher in the University of Adelaide (UoA). She is the receiver of several awards, including Women's Research Excellence Award by UoA. She has received over 4400 citations and h-index is 19.

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