Abstract

Borophene, a 2D allotrope of boron, exhibits several extraordinary properties, namely high specific surface area, metallic conductivity, high charge carrier mobility, anisotropy, electron-deficiency, etc., which are desirable for catalysis. Although several computational studies highlighted the potential of borophene-based catalysts, their experimental implementations are still limited. The experimental studies on borophene-based photocatalysts are rare, and only a few studies have employed borophene-based electrocatalysts for oxygen evolution reaction (OER). Moreover, their applicability towards sustainable strategies for H_2 generation, like external field-assisted OER and substituting OER by urea oxidation reaction (UOR), remains largely unexplored. Besides producing borophene via a facile sonochemical liquid phase exfoliation technique, its four novel and stable heterostructures, namely Pd nanoparticles-decorated borophene (Pd@B), reduced graphene oxide/Pd nanoparticles-anchored borophene (rGO/Pd@B), Au nanoparticles-supported borophene (Au@B) and cobalt phosphate/borophene (BCoPi) were developed. In Pd@B, borophene suppressed the agglomeration of Pd nanoparticles, and electron transfer from Pd to borophene generated $Pd^{\delta+}$ species, that stabilized its electron deficiency, resulting in a stable polarized heterostructure. Under visible light, it efficiently degraded the organic pollutants through the effective separation of charge carriers and the availability of multiple catalytic sites. The Pd@B also displayed reasonable electrocatalytic OER activity due to the active $Pd^{\delta+}$ sites for adsorption of OER intermediates. The integration of rGO with Pd@B enhanced the formation of $Pd^{\delta+}$ and created extended pathways for electron delocalization, that improved the OER activity (overpotential of 259 mV at 10 mA cm^{-2}), kinetics (Tafel slope of 59.17 mV dec^{-1}) and charge transfer resistance (R_{ct}) of rGO/Pd@B. Similarly, the electronic regulation in Au@B generated abundant $Au^{\delta+}$ sites, whereas borophene prevented the accumulation of Au nanoparticles and enabled efficient electron delocalization. It displayed better OER activity (overpotential of 270 mV at 10 mA cm^{-2}), faster kinetics (Tafel slope of 65.71 mV dec^{-1}) and lower R_{ct} than borophene. Moreover, it exhibited plasmonic properties, and borophene facilitated an effective separation of hot charge carriers, further boosting the OER activity. In BCoPi, borophene stabilized the OER-active higher valent Co species, modified the morphology and charge transport to enhance the activity and kinetics. To achieve 50 mA cm^{-2}, it demanded a low overpotential (337 mV) and exhibited a Tafel slope of 61.81 mV dec^{-1}. Utilizing urea as a sacrificial agent significantly reduced its potential requirement for UOR by 187 mV to attain 100 mA cm^{-2}, compared to OER. All the synthesized electrocatalysts demonstrated remarkable long-term durability towards OER/UOR performance. Moreover, all the developed catalysts displayed comparable and even superior performance to several recently reported 2D materials-based catalysts. Also, they were morphologically and chemically stable after prolonged catalytic reactions. Overall, this study demonstrates that the construction of suitable borophene-based heterostructures can enhance their stability and catalytic properties through intrinsic polarization and efficient delocalization of electrons, that can be utilized for energy conversion and environmental remediation.

Keywords: Borophene; Electrocatalysis; Heterostructure; Oxygen evolution reaction; Photocatalysis; Urea oxidation reaction.