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One-Pot Synthesis of Pd-based Metallenes for Energy Saving Hydrogen-Production

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Abstract : Hydrogen, recognized as a sustainable and pollution-free energy carrier, has garnered significant attention due to its potential to drive the transition to renewable energy systems. In this regard, electrolysis, a clean and efficient process for generating high-purity hydrogen and oxygen, offers a zero-CO_2 emission pathway for large-scale hydrogen production. However, among the emerging electrocatalyst materials, metallenes, a class of atomically thin 2D materials composed of metals and alloys, are gaining increasing attention due to their distinctive properties, including high surface area-to-volume ratios, excellent conductivity, and structural adaptability. This study explores the potential of metallenes—as an efficient electrocatalysts for energy-saving hydrogen production. This research focuses on synthesizing and characterizing Pd-based metallenes, particularly PdMo and PdMoNi. Electrochemical measurements were conducted using a three-electrode system in alkaline conditions, demonstrating the catalyst's superior performance in both Hydrogen Evolution Reaction (HER) and Oxygen Evolution Reaction (OER). Notably, Pd(0.03)MoNi(0.02) exhibited enhanced catalytic efficiency, achieving a cathodic current density of 10 mA/cm² at just 45 mV overpotential with a low Tafel slope, which is the indication of improved reaction kinetics. This study underscores the impact of Ni doping in PdMo metallenes, with evidence of enhanced electron transfer and structural integrity. For instance, XPS analysis reveals that the binding energy of Pd 3d in PdMo-Ni exhibits a 0.3 eV negative shift compared to PdMo. This chemical shift suggests that the electronic structure of Pd is altered due to electron transfer between Ni and Pd atoms. TEM images also demonstrate an increase in d-spacing from 0.231 nm in PdMo to 0.242 nm in PdMoNi, further indicating the structural changes due to Ni incorporation. X-ray diffraction (XRD) patterns were measured to analyze the crystal structures of PdMo and Ni-doped PdMo, the characteristic diffraction peaks at 38.1°, 46.7° and 68.1° correspond to the (111), (200) and (220) planes of the FCC phase of Pd (JCPDS NO. 46-1043), respectively with the addition of the Ni, these peaks become sharper, indicating enhanced crystallinity. The double-layer capacitance (Cdl) was determined by measuring the capacitive current related to double-layer charging at various scan rates (30, 60, 90, 120, and 150 mV/s) during cyclic voltammetry (CV). The Pd(0.03)MoNi(0.02) catalyst exhibits a Cdl of 0.13 mF/cm², indicating it has the largest effective electrochemical surface area (ECSA) among the other catalysts. This comprehensive investigation highlights metallenes as a promising class of electrocatalysts for clean hydrogen production. The work not only advances the understanding of metallenes synthesis and performance but also paves the way for future innovations in sustainable energy applications. By combining theoretical insights and experimental rigor, the findings contribute significantly to addressing global energy challenges through efficient and cost-effective hydrogen production technologies.

Keywords : electrocatalysis, green hydrogen, renewable Energy, 2D materials.
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