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Microwave-induced defective PdFe/C nano-electrocatalyst for highly efficient alkaline glycerol oxidation reactions

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Abstract

Pd-based mono- and bi-metallic nano-electrocatalysts (Pd/C and PdFe/C) have been synthesized using two different methods for comparison: conventional sodium borohydride (NaBH4) route and microwave-assisted reduction process. The performance of the nano-electrocatalysts is tested for glycerol oxidation reaction (GlyOR) in an alkaline medium. DFT simulation proves that incorporation of Fe to Pd(111) leads to an increased partial density of states (PDOS) compared to Pd alone, confirming the importance for bimetallic nano-electrocatalyst. The adsorption energy of glycerol onto PdFe is slightly weaker (A.E. = -48.89 eV) than the Pd alone (A.E. = -48.60 eV), indicating the ease with which glycerol can be generated at the PdFe surface than at the Pd alone. XRD show that microwave-irradiated samples (Pd(MW) and PdFe(MW)) are more crystalline than the conventional Pd and PdFe. TEM images show that the Pd(MW) and PdFe(MW) have slightly larger particle sizes (5.30 – 7.40 nm) than those from the conventional route (2.48 – 3.02 nm). Nitrogen adsorption-desorption analysis shows that the microwave samples exhibit slightly larger surface area compared to samples from NaBH4 route. Raman and XPS show that Pd(MW) and PdFe(MW) are more prone to defects (i.e., oxygen vacancies) compared to the NaBH4 route. The microwave samples gave the highest electrocatalytic properties toward glycerol than the NaBH4 route (including high electrochemical active surface area, high current density response, high resistance to poisoning due to carbonaceous intermediates arising from the GlyOR, and high conductivity or low interfacial resistance) compared to samples from the conventional NaBH4 method. The findings in this work go a long way to understanding the physico-chemical and electrochemical effects of microwave irradiation on bimetallic electrocatalyst for glycerol oxidation reaction, which open new opportunities for developing high-performance direct alkaline glycerol fuel cells.