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Multifunctional Pd-Sn Electrocatalysts Enabled by *In Situ* Formed SnO_x and TiC Triple Junctions

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Abstract

This paper describes an *in situ* formed, triple junction structured PdSn electrocatalyst dispersed on a stable conductive TiC surface. Through extensive characterization and computational modeling, we show that the multicomponent catalyst forms a unique PdSn/SnO_x/TiC triple junction structure. This structure stabilizes Pd and promotes its catalytic performance toward a model reaction, formic acid oxidation. Computational modeling suggests that the triple junction structure is the most stable configuration that provides desired anchoring sites for Pd and enables a favorable synergy between the multicomponents Pd, Sn, SnO_x, and TiC for high activity. The triple junction structure also can provide better stability against catalysts migration, detachment, or sintering. Experimental measurements also confirm that multicomponent catalysts provide synergistic functions. The intermediate products, CO_{ads}, prefer to adsorb onto the Pd sites, while the OH prefers the Sn and SnO_x sites, which function together to prevent catalyst poisoning.

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