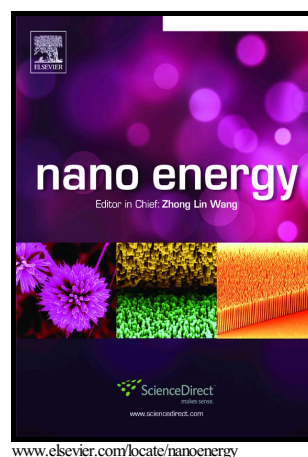


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Experimental Investigation and Theoretical Exploration of Single-Atom Electrocatalysis in Hybrid Photovoltaics: The Powerful Role of Pt Atoms in Triiodide Reduction

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ABSTRACT

Although single-atom catalysts (SACs) that bridge homogeneous and heterogeneous catalysis exhibit excellent performance in various reactions, only a few examples have reported the use of SACs in electrocatalysis, especially in new types of photovoltaics. This work focused on the association between SAC Pt₁/FeO_x and the electrocatalysis in hybrid photovoltaics, with the role of single-Pt atom in facilitating triiodide (I₃⁻) catalytic reduction and enhancing the conversion efficiency of dye-sensitized solar cells. Even with an extremely low dispersion density of one Pt atom per 100 nm² (the atomic ratio between Pt and Fe is 1:12214), the conversion efficiency could be enhanced by 69.3% compared to bare FeO_x. DFT calculation indicated that ionization potential (*IP*), which was responsible for the rate-determining step, decreased with the anchor of single-Pt atoms on an oxygen-terminated Fe₂O₃(001) slab, thereby the electron-donating ability of catalysts was enhanced. The interaction between I⁻ and O₃⁻ terminated Pt₁/Fe₂O₃(001) showed that charge transfer occurred mainly between I and Pt atoms. Single

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