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Graphical Abstract

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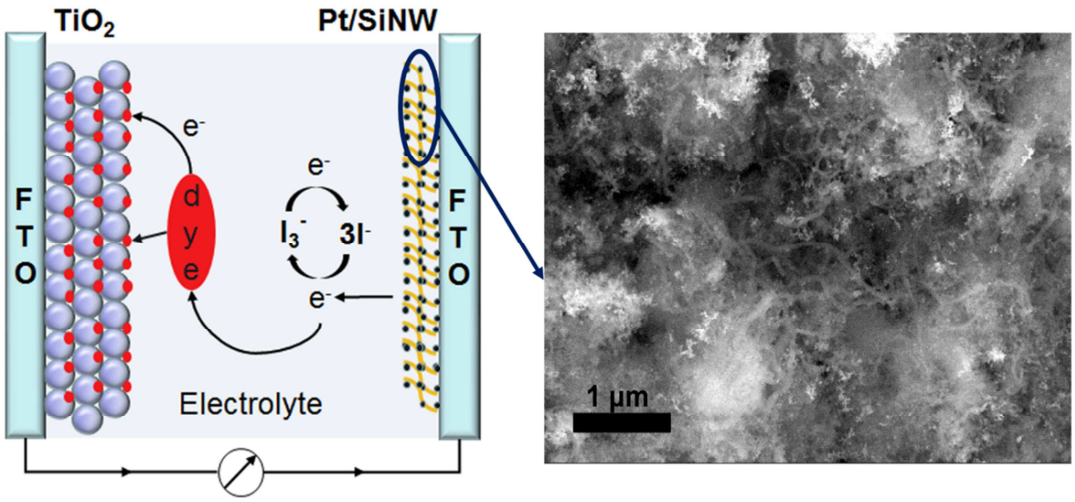

Pt nanoparticle/Si nanowire composites are employed as the counter electrode in dye-sensitized solar cells. Si nanowires prevent metal nanoparticles from agglomeration. The density functional theory calculation shows that the adsorption energy of I atom on the Pt/Si interface is -0.8 eV, which is the optimal adsorption energy for triiodide reduction. The power conversion efficiency of device based on the Pt/SiNW electrode is 3.8% higher than that of the device based on Pt.