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Organic Molecule-Functionalized Zn_3P_2 Nanowires for Photochemical H_2 Production: DFT and Experimental Analyses

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ABSTRACT

Hydrogen production via photochemical reactions in water/methanol solutions containing Zn_3P_2 nanowires functionalized with an organic molecular layer is shown to be between 217 and 405 times higher than that obtained in absence of the molecular layer. Combined surface characterization and theoretical analyses are used to elucidate aspects of the photochemical reaction process. It is found that the protective layer exerts a passivation role decreasing the rate of nanowire degradation, while facilitating electron transfer for the hydrogen evolution reaction.

Keywords: Hyudrogen production, density functional theory, functionalized nanowires