

Title: *Structural, mechanical, electronic and optical properties of Si decorated zinc oxide nanotube photocatalyst for hydrogen evolution via overall water splitting: A DFT study*

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Abstract: This work investigated an Si-doped single-walled [zinc oxide nanotube](#) (SWZnONT) as [photocatalyst](#) for [hydrogen energy](#) production. [Photocatalytic](#) properties of the Si-doped SWZnONT were determined based on analysis of structural, electronic and [optical absorption](#) spectra using [density functional theory](#). The obtained data for structural and mechanical properties of the systems revealed that Si-doped SWZnONT was stable under 2.7 % and 5.5 % of Si concentrations. Furthermore, the studied [SWZnONT doped](#) with 2.7 % Si demonstrated an indirect band gap of 2.6 eV which is desirable to be an ideal [photocatalyst](#). Results from [optical spectra](#) analysis revealed that Photo-generated holes on the Si-doped SWZnONT surface promote water splitting.

Keywords: Si-doped ZnO nanotube Single-walled zinc oxide nanotube (SWZnONT) Density functional theory (DFT) Photocatalysis Hydrogen production

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