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.

Keyword: Photocatalyst, Zinc Oxide Nanotubes, Water Splitting, Hydrogen Energy, Overpotential

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