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First-Principles Study of Zn-Site Transition Metal Doping in ZnSnO3 for Enhanced Performance in Dye-Sensitized Solar Cells (DSSCs)

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Zinc stannate ($ZnSnO_3$) is a wide-bandgap oxide semiconductor with considerable potential for application in solar energy conversion devices, such as dye-sensitized solar cells (DSSCs). However, its practical use is limited by its low visible spectrum absorption. The current study investigates the Zn-site partial doping with transition metals specifically Cu, Ni, and Co effect on the electronic structure and optical absorption properties of orthorhombic $ZnSnO_3$ using first-principles density functional theory (DFT). Zn-site doping was utilized owing to its superior ionic compatibility and reduced formation energy. The results obtained indicated that doping with transition metals significantly narrows the bandgap and generates shallow electronic states near the canter of the valence and conduction bands, hence enhancing light harvesting. Optical property calculations utilizing the complex dielectric function showed a red shift in the absorption edge and a general increase in absorption intensity across the visible spectrum from Cu-doped systems showing the most notable change. This computational effort provides a theoretical foundation for creating $ZnSnO_3$ photoanode materials with enhanced light absorption and electrical performance for future solar-energy systems.

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