Contribution ID: **41** Type: **not specified**

DFT analysis of structural, electronic and optical properties of Ni and Zn doped CoS counter electrode for dye sensitized solar cells

Friday, 21 November 2025 11:00 (15 minutes)

In this study, first principles calculations are employed to investigate the structural, electronic, and optical properties of (Ni, Zn)xCo1−xS in its tetragonal phase. The optimized lattice parameters and negative defect formation energies confirm structural integrity and thermodynamic stability across doping levels. The calculations are performed using both the GGA and the HSE06 hybrid functional, ensuring an accurate description of electronic band structure. The system retains a direct band gap in all doped configurations, with a systematic reduction upon doping most pronounced in the co-doped case, demonstrating effective band gap engineering. Ni doping enhances electron localization through stronger Ni–S bonding, while Zn doping promotes electron delocalization, collectively improving charge transport. The band edges are dominated by hybridized Co(3d), Ni(3d), and S(3p) states, with Zn(4s) modulating valence band characteristics. A notable reduction in the effective masses of electrons and holes upon co-doping indicates enhanced carrier mobility and improved conductivity. Optical calculations reveal increased dielectric constant, strong absorption in the UV–visible range, and enhanced electrical conductivity, particularly in co-doped systems. These results establish (Ni, Zn)xCo1−xS as a highly tunable, stable, and efficient material, positioning it as a promising low-cost alternative to platinum-based counter electrodes in dye-sensitized solar cells. Moreover, this work offers crucial guidance for experimentalists in tuning CoS properties via doping for efficient dye sensitized solar cells.

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Session Classification: Friday Morning II

Track Classification: AfPS