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“Green”Aqueous Synthesis, Structural and Optical Properties of Quaternary Cu_2ZnSnS_4 and Cu_2NiSnS_4 Nanocrystals

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Elemental substitution in Cu_2ZnSnS_4-like chalcogenides opens up the potential to create alternative low-cost photovoltaic and thermoelectric materials with tunable properties. The method of “green” synthesis in aqueous solutions, based on the protocol previously proposed for CZTS [1], has been used to obtain Cu_2NiSnS_4 (CNTS) nanocrystals (NC). This method opens up possibilities for non-toxic, economical large-scale production.

The structural and optical properties of CXTS NCs (X = Ni, Zn) NCs were studied in colloidal solutions and thin films. Thin films of NCs were deposited on glass substrates by spin coating method. From X-ray diffraction (XRD) and Raman spectroscopy data, it was concluded that the synthesised NCs of CZTS and CNTS with sizes in the range of 1.5 to 2.5 nm are likely to have a kesterite structure with disordered cations. CNTS shows broader diffraction and Raman peaks, indicating a higher degree of cationic disorder than in CZTS. The theoretical calculation of Raman peaks was carried out using the tight binding method to better understand the effect of cationic disorder on Raman spectra. The calculations qualitatively agree with the experimental results. CZTS and CNTS films between 40 and 150 nm thick were prepared from colloidal solutions demonstrating the versatility of the material and its compatibility with thin film deposition techniques. The thickness of the thin films was determined from atomic force microscopy (AFM) and spectroscopic ellipsometry (SE) data. AFM height profiles of low aggregated NCs show an average size in line with XRD analysis. Optical absorption studies of NCs reveal a continuous spectrum in the visible range with a bandgap of approximately 2.2 ± 0.3 eV for both materials positioning them as effective absorbers for solar cell applications. Absorption coefficients for both exceed 10^2 cm^{-1} at 700 nm and reach over 10^4 cm^{-1} at 400 nm indicating significant light-absorbing capabilities of the material.
These properties highlight the versatility of CNTS and demonstrate the advantages of “green” synthesis methods for the development of sustainable, low-cost nanomaterials for energy applications.[2]

Type of presence

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