

# “Green” Aqueous Synthesis, Structural and Optical Properties of Quaternary $\text{Cu}_2\text{ZnSnS}_4$ and $\text{Cu}_2\text{NiSnS}_4$ Nanocrystals

Tuesday, November 5, 2024 3:20 PM (15 minutes)

Elemental substitution in  $\text{Cu}_2\text{ZnSnS}_4$ -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  $\text{Cu}_2\text{NiSnS}_4$  (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  $2.2 \pm 0.3$  eV for both materials positioning them as effective absorbers for solar cell applications. Absorption coefficients for both exceed  $10^2$   $\text{cm}^{-1}$  at 700 nm and reach over  $10^4$   $\text{cm}^{-1}$  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

**Primary author:** Ms IVAKHNO-TSEHELNYK, Oleksandra (Semiconductor Physics & Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology)

**Co-authors:** Dr SELYSHCHEV, Oleksandr (Semiconductor Physics & Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology.); Prof. KONDRATENKO, Serhiy (Taras Shevchenko National University of Kyiv); Prof. DZHAGAN, Volodymyr (Lashkaryov Institute of Semiconductor Physics (ISP), NAS of Ukraine); HERTLING, Lukas (Semiconductor Physics & Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology); Prof. RT ZAHN, Dietrich (Semiconductor Physics & Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology)

**Presenter:** Ms IVAKHNO-TSEHELNYK, Oleksandra (Semiconductor Physics & Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology)

**Session Classification:** Workshop on Sustainable Materials and Technologies

**Track Classification:** Workshop on Sustainable Materials and Technologies