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Title: Tailoring Crystal Structures of $Cu_2ZnGe_xSn_{1-x}S_4$ for Advanced Photovoltaic Applications
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Topic I : Nanomaterials and Functional Nanostructures

T1-P15

Tailoring Crystal Structures of $Cu_2ZnGexSn1-xS_4$ for Advanced Photovoltaic Applications

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Abstract

Quaternary chalcogenides are promising absorber materials for thin-film photovoltaic devices due to their earth-abundant composition, tunable band gaps, and favorable optoelectronic properties. In this work, we investigate the structural and thermodynamic evolution of $Cu_2ZnGexSn_1-xS_4$ ($0 \leq x \leq 1$) using first-principles density functional theory (DFT) within the full-potential linearized augmented plane-wave method. Our calculations demonstrate a composition-driven phase transition: the tetragonal stannite phase is stable for Sn-rich alloys, while increasing Ge concentration stabilizes the orthorhombic wurtzite-stannite phase beyond ~80% Ge substitution. This behavior is confirmed by enthalpy of formation and Gibbs free energy analyses, which show that the transition is governed by cation size effects and is largely independent of temperature and pressure. Furthermore, lattice parameters decrease with Ge incorporation, following Vegard's law, accompanied by a reduction in unit cell volume. These results provide fundamental insights into phase stability in $Cu_2ZnGexSn_1-xS_4$ alloys and underline the role of cation substitution in tuning crystal structures. Such knowledge is crucial for guiding the design of next-generation photovoltaic absorbers with enhanced stability and efficiency.

Keywords: $Cu_2ZnGexSn_1-xS_4$ (CZGTS), Density Functional Theory (DFT), Phase transition, Quaternary chalcogenides, Photovoltaic absorbers

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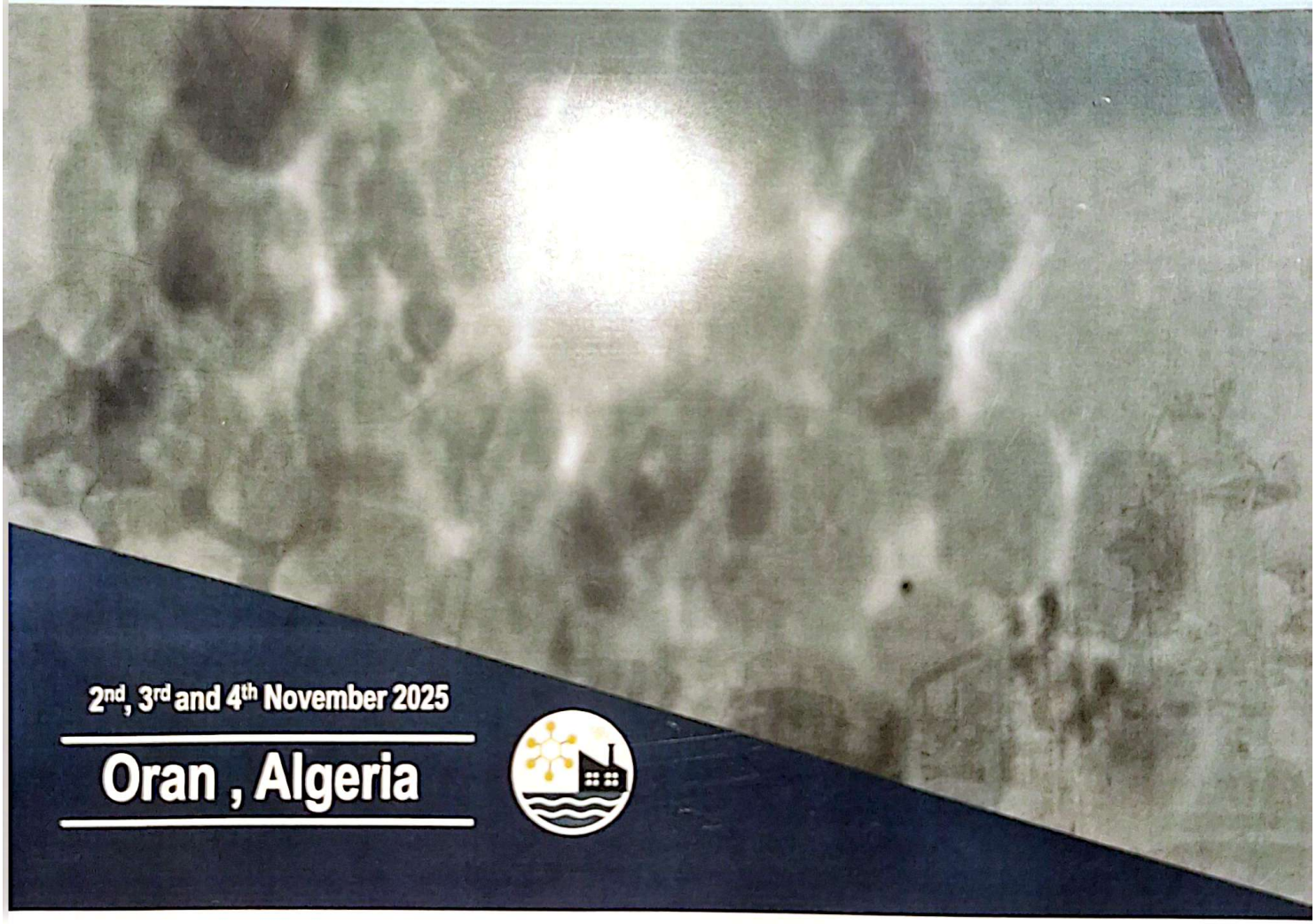
Abstract Book



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