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**A Study of Structure and Electronic Properties of Chalcopyrites Semiconductor Invoking Density Functional Theory**

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**Abstract**

Ternary chalcopyrites, having general formula AIBIIIC2, are of considerable research interest due to their optoelectronic applications as solar energy converters, nonlinear optical devices, light emitting diodes and detectors. In this study, an attempt has been made to correlate optoelectronic properties of CuTiX2 (X = S, Se and Te) with computed Density Functional Theory based electronic descriptors. The ground state configurations and low lying isomers of CuTiX2 (X = S, Se and Te) are analyzed invoking electronic structure theory. Our computed HOMO-LUMO energy gap (2.405 eV–3.197 eV) signifies CuTiX2 as potential candidate for solar cell applications. CuTiS2 and CuTiTe2 exhibit the maximum and the minimum energy gap respectively. HOMO-LUMO energy gap maintains an expected trend with DFT based global descriptors. A close agreement between our computed results and experimental data establishes the importance of present study.

**Keywords:**

Density functional theory, Chalcopyrite semiconductor, Descriptors, Solar cells

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