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## **INVESTIGATION OF PROPERTIES OF MATERIALS USED FOR SOLAR PHOTOVOLTAIC CELLS AND APPLICATIONS OF THE SOLAR CELLS**

The present thesis is devoted to search of materials for solar cells among the ternary semiconducting compounds  $\text{CuXY}_2$  ( $X = \text{Al, Ga and In; Y = S and Se}$ ). The energy band gaps, dielectric constants and absorption coefficients which decide the fate of solar materials have been thoroughly investigated.

Going beyond the identification of best possible solar cell materials among semiconductor chalcopyrites, the required solar panel cross-section area to meet out electrical power necessities of a middle class house has been calculated and presented.

The electronic and optical properties of the  $\text{CuXY}_2$  chalcopyrite semiconductors have been computed using linear combination of atomic orbitals (LCAO) method within density functional theory (DFT) and also by using full potential linearized augmented plane wave (FP-LAPW) method with different types of generalized gradient approximations (GGA). From the energy band computations, it is seen that these materials are direct band gap semiconductor at  $\Gamma$  point. The computed band gaps have been compared with the available experimental and theoretical



data. Except fine structures, overall topology of energy bands is found to be in fair agreement with available data. The optical properties such as dielectric tensors, reflectivity, refractive index and absorption coefficients for these materials are computed using LCAO and FP-LAPW schemes. Different characteristic peaks found in the dielectric tensor components for these materials are successfully interpreted in terms of interband transitions within the energy bands. The calculated peaks are found to be in good agreement with the available experimental data using spectroscopic ellipsometry. Wherever required, *ad hoc* scissor corrections have been used within the FP-LAPW calculations. Except amplitude of absorption coefficients in different computations (which may be due to common multiplicative factor), the overall shape of absorption coefficients, refractive index and reflectivity data are found to be in tune with the available experimental results.

The main objective of the present investigations is to select the most appropriate materials among the chalcopyrites compounds which may have the highest absorption capacity and efficiency in order to reduce the cross-sectional area and hence cost indulged in manufacturing of solar photovoltaic panel for practical applications. Therefore, a detailed comparison of the energy band gaps, overall absorption capacity, reported energy conversion efficiency and effects of atmospheric conditions on the present series of chalcopyrites have been presented. The results show that  $\text{CuGaSe}_2$  and  $\text{CuInSe}_2$  are more suitable chalcopyrites for fabrication of solar cell than  $\text{CuGaS}_2$ ,  $\text{CuInS}_2$ ,  $\text{CuAlS}_2$  and  $\text{CuAlSe}_2$ . Keeping the environmental issues (intermediate toxicity) in mind, it is concluded that  $\text{CuInSe}_2$  is the most promising and can be used for the construction of solar panels at both small and large scales.