

# Quadrupole Interaction in Ternary Chalcopyrite Semiconductors: Experiments and Theory

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Electric field gradients have been measured at substitutional lattice sites in ternary semiconductors using Perturbed  $\gamma$ - $\gamma$  Angular Correlation spectroscopy (PAC). The experimental results for  $A^I B^{III} C_2^{VI}$  chalcopyrite structure compounds and  $\square A^{II} B_2^{III} C_4^{VI}$  defect chalcopyrites are compared with ab-initio calculations. The latter were carried out with the WIEN code that uses the Full Potential Linearized Augmented Plane Wave method within a density functional theory. The agreement between experiment and theory is in most cases very good. Furthermore, the anion displacements in  $AgGaX_2$ -compounds (X: S, Se, Te) have been determined theoretically by determining the minimum of the total energy of the electrons in an elementary cell.

*Key words:* Quadrupole Interaction; Chalcopyrite Semiconductors; First Principles Calculations; Perturbed Angular Correlations; Structure Parameters.