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Coupling coefficients and excitonic transitions in CuGaSe₂

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Abstract content
   (Max 300 words)
Formatting &
Special chars

The chalcopyrite structure contains semiconductor compounds and alloys that crystalize in a space group D_{2d}¹². These compounds are used in the fabrication of solar cells.
The excitonic radiative transitions in chalcopyrite CuGaSe<sub>2/<sub> are investigated using group theoretical methods in the absence and presence of spin-orbit interaction. We have calculated the coupling coefficients for optical direct transitions at high symmetry points Γ, X, N and P in the Brillouin zone of chalcopyrite structure. The inclusion of spin-orbit interactions results in modification of selection rules for radiative processes. The obtained dielectric functions,tensors, absorption coefficients and refractive index are determined by the exciton symmetry &Gamma<sub>6x&Gamma₆, &Gamma<sub>6x&Gamma₇ and &Gamma₇x&Gamma₇ Kronecker products. The critical point analysis throughout the Brillouin zone at point &Gamma, X, N, and P are discussed in the absence and presence of spin-orbit interaction in the study of reflectivity peaks. The theoretical results are used in the interpretation of reflectivity and photoluminescence spectra in chalcopyrite group and coupling coefficients also useful in the construction of effective Hamiltonains from which estimates of optical transition energies can be made.

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PhD

Main supervisor (name and email)
and his / her institution

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