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Coupling coefficients and excitonic transitions in CuGaSe_2

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Abstract content
 (Max 300 words)
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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_2 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 Γ_{6x} , Γ_{6-} , Γ_{6x} , Γ_{7-} and Γ_{7-x} , Γ_{7-} Kronecker products. The critical point analysis throughout the Brillouin zone at point Γ , 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 Hamiltonians from which estimates of optical transition energies can be made.

Apply to be considered for a student award (Yes / No)?

No

Level for award (Hons, MSc, PhD)?

PhD

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

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Would you like to submit a short paper for the Conference Proceedings (Yes / No)?

Yes

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