

Effects of cation substitution in the vibrational spectra of colloidal ternary and quaternary chalcogenide nanocrystals

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Compounds of ternary (I-III-VI) and quaternary (I-II-IV-VI) metal chalcogenide nanocrystals (NC) are promising materials for photodetectors and absorber layers of thin-film solar cells of the new (third) generation, fluorophores and low-toxic fluorescent labels for biomedical applications, photocatalytic devices, supercapacitors, and other energy conversion and storage devices. The advantages of these compounds are the cheap and non-toxic components, as well as the possibility of partial substitution of any of the elements, which allows the properties of the material to be modified in a wide range. These materials are characterized by a combination of several important physical parameters, such as high optical absorption coefficient (10^{4-5} cm⁻¹), the spectral position of the absorption edge in the range of solar radiation (~1.5 eV for bulk material), good electrical and thermal conductivity, advantageous position of the band edges in terms of charge transfer to other components.

The phonon spectra of I-III-VI and I-II-IV-VI NCs were little studied, because the crystal structure and component composition of these compounds significantly depend on the technological conditions of production. Even among the available data, there were inconsistencies in interpretation.

Here are presented phonon Raman spectra of ternary NC Me-In-S (Me = Cu, Ag, Hg) and quaternary Me-Zn-Sn-S (Me = Cu, Ag) and all potential secondary phases, depending on their component composition.

Topics

Session A. Physics of condensed matter and spectroscopy

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