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Electronic and optical properties of Cu_2XS_3 (X=Si, Ge, Sn): prospects for photovoltaics

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Abstract:

Theoretical study of structural, electronic and optical properties of Cu_2XS_3 (X=Si, Ge, Sn) ternary compounds, which could be easily fabricated using modern epitaxial techniques, has been performed by means of *ab initio* DFT calculations in order to find cheap and environment friendly materials applicable in photovoltaics. To obtain the more realistic physical values the modified Becke-Johnson potential has been applied to the calculations. The different phases were considered: two hexagonal, two orthorhombic and one monoclinic. The latter one was determined to be the most stable for all compounds. It was found for all Cu_2XS_3 family that increase of the number of IV group element always leads to the increase of lattice constants by about 3–5% and the unit cell volume up to 10%.

The electronic properties demonstrate the semiconducting nature of Cu_2XS_3 compounds considered for monoclinic phase and two orthorhombic phases. Moreover, Cu_2SnS_3 is practically gapless. Both hexagonal phases seem to lead to a metallic behavior. Cu_2XS_3 compounds in monoclinic phase are found to be direct-gap semiconductors with the band gap values of 1.72, 0.46 and 0.03 eV for Cu_2SiS_3, Cu_2GeS_3 and Cu_2SnS_3, respectively, following the tendency of decreasing the band gap with increasing of the IV group element.

The imaginary (ε_2) and real (ε_1) parts of dielectric function for Cu_2XS_3 compounds demonstrate small differences between light polarizations along *a* and *c* directions which strongly differ from the one along *b* direction. This may be explained by the fact that the *a* and *c* lattice constants practically coincide being two times smaller than *b* lattice constant. The static dielectric function $\varepsilon_1(0)$ remains practically the same for different light polarizations up to 2 eV and looks more anisotropic at higher energies, having the smaller values (~7) for Si- and the larger values (~14) for Sn-containing material.

Cu_2XS_3 compounds show absorption coefficients greater than 10^5 cm^{-1} above their respective band gaps making them suitable for energy conversion of the solar spectrum. Relying on obtained results, Cu_2SiS_3 or $Cu_2Si_{1-x}Ge_xS_3$ solid solutions (if achievable experimentally) seems to be promising materials for photovoltaic applications.