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Crystallographic, optical, and electronic properties of (Cu,Li)InS₂ system

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Abstract

To investigate the effect of a lithium doping in chalcopyrite-type CuInS₂ on its crystallographic and optical properties, we prepared (Cu,Li)InS₂ samples by a mechanochemical process and post-heating at 550°C in H₂S gas. The single-phase chalcopyrite-type (Cu_{1-x}Li_x)InS₂ solid solution could be obtained for the samples with $0.0 \leq x \leq 0.10$. The lattice constants a and c of tetragonal chalcopyrite-type (Cu_{1-x}Li_x)InS₂ solid solution increase with increasing Li content. The band gap energy of the (Cu_{1-x}Li_x)InS₂ solid solution linearly increased from 1.44 eV of CuInS₂ ($x = 0.0$) to 1.54 eV of (Cu_{0.90}Li_{0.10})InS₂ ($x = 0.10$). We performed first-principles band structure calculations for chalcopyrite-type (Cu_{1-x}Li_x)InS₂, using the HSE06 nonlocal screened hybrid density functional. Theoretically, the band-gap energies of the (Cu_{1-x}Li_x)InS₂ increase with increasing Li content. The energy levels of the valence band maxima (VBMs) were estimated from the ionization energy measured by photoemission yield spectroscopy. The ionization energy of chalcopyrite-type (Cu_{1-x}Li_x)InS₂ solid solutions increased from 5.45 eV of CuInS₂ ($x = 0.0$) to 5.79 eV of (Cu_{0.90}Li_{0.10})InS₂ ($x = 0.10$). The energy level of the VBM of the (Cu_{1-x}Li_x)InS₂ solid solution considerably decreases with increasing Li content, x . The conduction band minimum (CBM) level of the (Cu_{1-x}Li_x)InS₂ solid solution also decreases with increasing Li content. The Li-doping in CuInS₂ is expected to be useful for decreasing the VBM of CuInS₂ absorber and increasing the band-gap energy of CuInS₂ absorber without increasing the CBM level.

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