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Effects on magnetic properties and light absorption bandgaps of lattice distortions in $CuIn_{1-x}Co_xSe_2$ chalcopyrites

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Abstract: Co doped $CuInSe_2$ compounds have been synthesized by vacuum arc melting-vacuum solid sintering- mechanical milling technology, and their crystal structures, magnetic and light absorption properties have been systematically investigated by using X-ray diffraction, vibrating sample magnetometer and UV-Vis spectrophotometer. X-ray diffraction analyses show that $CuIn_{1-x}Co_xSe_2$ (x=0-0.2) crystallize in tetragonal chalcopyrite structure with a space group of $I\bar{4}2d$. Co partly substitutes for In at the 4b site. The studies of magnetic properties show that $CuIn_{1-x}Co_xSe_2$ (x=0.1-0.3) show supermagnetic characteristics at room temperature with applying an external field. Co doping can adjust the light absorption bandgaps of $CuIn_{1-x}Co_xSe_2$ from 1.25 to 1.53eV. These phenomena are revealed to be closely correlated with the lattice distortions induced by Co doping into $CuInSe_2$. The magnetism of Co doped $CuInSe_2$ is suggested to come from the double-exchange mechanism. The magnetic moment and light absorption bandgap depend upon the lattice distortions of (In,Co)Se4 and CuSe4 tetrahedrons, it shows that the magnetic moment is going up with the increase of Se-(In,Co) bond length and the decrease of (In,Co)-Se-(In,Co) bond angle; the light absorption bandgap is going up with the increase of volume distortion of CuSe4 tetrahedron.

Key word: lattices distortion, double exchange, strong relation

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