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Tai Wang, Yongguan Guo, Cong Wang, Shuowang Yang

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Effects on magnetic properties and light absorption bandgaps of

lattice distortions in CuIn_{1-x}Co_xSe₂ chalcopyrites

Tai Wang, Yongquan Guo^{a)}, Cong Wang, Shuowang Yang

School of Energy Power and Mechanical Engineering, North China Electric Power

University, Beijing 102206, China

Abstract: Co doped CuInSe2 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_xSe₂ (x=0-0.2) crystallize in tetragonal chalcopyrite structure

with a space group of $\overline{142}$ d. Co partly substitutes for In at the 4b site. The studies of magnetic

properties show that CuIn_{1-x}Co_xSe₂ (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_xSe₂ from 1.25 to 1.53eV. These phenomena are revealed to be closely

correlated with the lattice distortions induced by Co doping into CuInSe₂. The magnetism of

Co doped CuInSe₂ 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

a) author to whom correspondence should be addressed Email: yqguo@ncepu.edu.cn; Tel:

+86-10-61772853; Fax: +86-10-61772383

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