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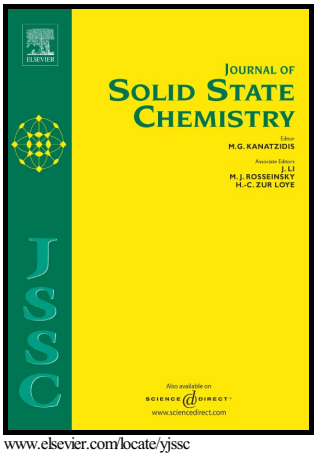

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PII: S0022-4596(17)30099-3
DOI: http://dx.doi.org/10.1016/j.jssc.2017.03.018
Reference: YJSSC19722

To appear in: *Journal of Solid State Chemistry*

Received date: 23 January 2017
Revised date: 23 March 2017
Accepted date: 25 March 2017

Cite this article as: Marcel Quennet, Anna Ritscher, Martin Lerch and Beate Paulus, The order-disorder transition in Cu_2ZnSnS_4: A theoretical and experimental study, *Journal of Solid State Chemistry* http://dx.doi.org/10.1016/j.jssc.2017.03.018

The order-disorder transition in Cu_2ZnSnS_4: A theoretical and experimental study

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Abstract

In this work the Cu/Zn order-disorder transition in Cu_2ZnSnS_4 kesterites on Wyckoff positions 2c and 2d was investigated by a structural and electronic analysis in theory and experiment. For experimental investigations stoichiometric samples with different Cu/Zn order, annealed in the temperature range of 473-623 K and afterwards quenched, were used. The optical gaps were determined using the Derivation of Absorption Spectrum Fitting (DASF) method. Furthermore, the order-disorder transition was examined by DFT calculations for a closer analysis of the origins of the reduced band gap, showing a good agreement with experimental data with respect to structural and electronic properties. Our studies show a slight increase of lattice parameter *c* in the kesterite lattice with increasing disorder. Additionally, a reduced band gap was observed with increasing disorder, which is an effect of newly occurring binding motifs in the disordered kesterite structure.

Keywords: CZTS, order-disorder transition, cation distribution, kesterites, electronic structure, DFT

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