Ground state of spin chain system by Density Functional Theory

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Abstract: The Cu-O based spin chain system A_2CuO_3 (A = Sr, Ca) has attracted considerable attention of scientists during the last decades due to its unique electronic structure. This paper presents a ground state optimization for the periodic structure of Ca_2CuO_3 using the Density Functional Theory (DFT). The electronic structure analysis was carried out on the basis of cell optimization using the PBE functional with DNP basis set. Until now, the numerical results were obtained only with exclusion of CaO bilayers from full ab initio treatment. We demonstrate here that the correct covalent insulating ground state may be obtained if the antiferromagnetic interaction along the spin chain is included. The best estimated band gap is 0.79 eV. We also show that the CaO bilayers sufficiently contributed to the distribution of d-states above Fermi level.

Author Keywords: Ab initio; Antiferromagnet; Ca_2CuO_3; DFT; Ground state; Spin chain

Source title: Computational Materials Science
Link: Scorpus Link
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ISSN: 9270256
CODEN: CMMSE
DOI: 10.1016/j.commatsci.2010.04.002
Language of Original Document: English
Abbreviated Source Title: Computational Materials Science
Document Type: Article in Press
Source: Scopus
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