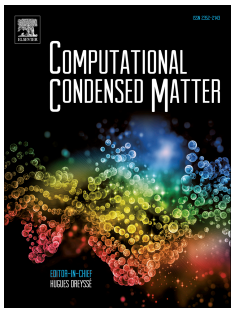
Accepted Manuscript



The effects of chemical bonding on the topological property of half-Heusler compounds: First principle calculation

C. Li, Y.F. Zhao, B.Q. Chi, Y.Y. Gong, C.Q. Sun

PII: S2352-2143(14)00003-3

DOI: 10.1016/j.cocom.2014.08.002

Reference: COCOM 2

To appear in: *Computational Condensed Matter*

Received Date: 2 July 2014

Revised Date: 1 August 2014

Accepted Date: 18 August 2014

Please cite this article as: C. Li, Y.F. Zhao, B.Q. Chi, Y.Y. Gong, C.Q. Sun, The effects of chemical bonding on the topological property of half-Heusler compounds: First principle calculation, *Computational Condensed Matter* (2014), doi: 10.1016/j.cocom.2014.08.002.

The effects of chemical bonding on the topological property of half-Heusler compounds: first principle calculation

C. Li,[a] Y. F. Zhao,[a] B. Q. Chi,[b] Y. Y. Gong,[a]* and C. Q. Sun[a,c]

[a] Center for Coordination Bond Engineering, Department of Materials Science and Engineering, China Jiliang University, China

[b] College of Modem Science and Technology, China Jiliang University, China

[c] School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore

E-mail: canli1983@gmail.com

Abstract

The dependence of ($E_{\Gamma 6}$-$E_{\Gamma 8}$) on the lattice constants has been studied for four half- Heusler compounds. First principle simulation was carried out to calculate the electronic structure and the obtained results were compared among different compounds. It is found that the change of ($E_{\Gamma 6}$-$E_{\Gamma 8}$) with strain exhibits opposite trend for III-VIII-V half- Heusler compounds and II-VIII-VI half- Heusler compounds. Moreover, for III-VIII-V half- Heusler compounds the valent orbital are usually fixed and the conduct orbital move away from Fermi level, whereas for II-VIII-VI half-Heusler compounds the conduct orbital tend to be fixed and the valent orbital move away from Fermi level as the lattice constant is reduced. The different trends of the variation of electronic structures are caused by the different extra-nuclear electrons of IIA and IIIB group elements which change their chemical bonding.

Keywords: half-Heusler compounds; topological insulator; electronic structure; first principle calculation.