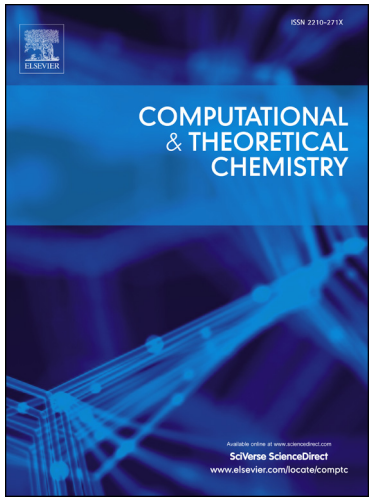

First-principles Calculation of Structural, Electronic, and Optical Properties of Wurtzite-stannite $Cu_2MgSi(S_xSe_{1-x})_4$ Alloys

Dan Li, Furi Ling

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First-principles Calculation of Structural, Electronic, and Optical Properties of Wurtzite-stannite $Cu_2MgSi(S_xSe_{1-x})_4$ Alloys

Dan Li [a,*], Furi Ling [b]

[a] School of Physics and Electronics Information, Hubei University of Education, Wuhan 430205, China

[b] School of Optical and Electronic Information, Huazhong University of Science and Technology, Wuhan 430074, China

Abstract

The structural, electronic, and optical properties of wurtzite-stannite $Cu_2MgSi(S_xSe_{1-x})_4$ alloys have been calculated based on Heyd-Scuseria-Ernzerhof (HSE) screened hybrid functional. The calculated band gap bowing parameter is 0.164 eV which may be a good reference for future research. According to the calculations of the density of states, we find that the peaks in the conduction band have a tendency of shifting to the lower energy as S concentration decreases. Furthermore, the dielectric function, reflectivity, and absorption coefficient are presented and discussed in detail. The spectra of dielectric function shift to lower energy region with the decrease of the S concentration. The static dielectric constants increase with the decrease of S mole fraction. And the strength of absorption peaks almost decrease. The absorption edge and the peak in the reflectivity have a tendency of shifting to lower energy.

* Corresponding author. Tel./fax: +86 27 87793023.
E-mail address: 417218520@qq.com (D. Li).