

CuInS₂晶体结构预测及电子结构性质

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Prediction of Crystal structure and electronic structure of CuInS₂

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摘要 图/表 参考文献 相关文章 (0)

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摘要 利用基于多目标粒子群优化算法的卡里普索(CALYPSO)软件预测了CuInS₂晶体在常压下的结构。结果表明CuInS₂晶体在常压下为四方晶系,空间群为I-42 d。计算了CuInS₂晶体的弹性常数矩阵,得到的弹性常数满足了晶体的机械稳定型条件。通过弹性常数计算了体模量,杨氏模量和剪切模量。最后,分别用杂化泛函方法计算了CuInS₂的能带结构和投影态密度,结果显示CuInS₂晶体为直接带隙半导体,带隙为1.22 eV。为了进一步分析CuInS₂晶体的性质,计算了电荷密度和电子局域函数。结果显示,Cu在CuInS₂中的成键过程发生了电荷转移,Cu原子和S原子之间是共价键为主,In原子和S原子之间是离子键为主。

关键词 : CuInS₂晶体, 结构预测, 电子结构, 化学键

Abstract : The structure of CuInS₂ crystal at 0 GPa was successfully predicted by using the CALYPSO software in developed particle swarm optimization algorithm. The result shows that the CuInS₂ crystal under atmospheric pressure is a tetragonal crystal system, and its space group is I-42 d. The elastic constant matrix of the CuInS₂ crystal was calculated, and the obtained elastic constant meets the mechanical stability conditions of the crystal. On the basis of the elastic constant, the volume modulus, young's modulus and shear modulus were calculated. Finally, the hybrid functional method was used to calculate the band structure of CuInS₂ and projection state density, respectively. The results show that the CuInS₂ crystal is a direct band gap semiconductor with a band gap of 1.22 eV. In order to further analyze the properties of the CuInS₂ crystal, the charge density and electron local function were calculated. The results show that the Cu bonding process in CuInS₂ has charge transfer, the covalent bonding is between Cu atom and S atom and the ionic bonding is between In atom and S atom.

Key words : CuInS₂ crystal predicted structure electronic structure chemical bond

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