材料合成及性能

Zn空位及Cu掺杂对ZnTe电子结构及光学性质的影响

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摘要： 利用基于密度泛函理论框架下的平面波赝势法和广义梯度近似,计算分析了ZnTe结构本体、掺入杂质Cu ($Zn_{0.875}Cu_{0.125}Te$)及Zn空位($Zn_{0.875}Te$)体系的晶格常数及缺陷形成能,得到了不同体系的态密度、能带 结构、集居数、介电函数、损失函数、吸收光谱、光电导率、复折射率及反射率。结果表明,掺杂Cu和Zn空位对ZnTe的晶胞参数、能带结构以及光学性质都产生了一定程度的影响。由于空位及杂质能级的引入,缺陷体系体积减小,晶胞参数也产生了一定的改变,同时缺陷体系禁带宽度减小并给受主能级价带顶提供n型电导性;此外,缺陷体系吸收光谱产生红移,电子在可见光区的跃迁明显增强并出现介电峰,改善了ZnTe的光学性质。

关键词： ZnTe 第一性原理 电子结构 光学性质

Effects of Zn Vacancy and Cu-doping Impurity on Electronic Structure and Optical Properties in ZnTe

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Abstract: Calculation and detailed analysis were carried out to investigate the lattice parameter and defect formation energy of perfect zinc blend ZnTe, that with impurity $Cu(Zn_{0.875}Cu_{0.125}Te)$ and that with Zn vacancies ($Zn_{0.875}Te$) using the plane-wave ultrasoft pseudopotential method based on density function theory and generalized gradient approximation. We obtained the band structure, density of states,Mulliken populations, dielectric function, absorption spectrum, refractive index, reflectivity, optical conductivity and loss function of the three systems. The results show that Zn vacancy and Cu impurity have certain influence on the lattice parameters, energy band structure and optical properties. The volumes of defect systems decrease and the lattice parameters are changed to some extent compared to perfect ZnTe. The band gap decreases, providing a n-type conductivity to the top of the valence band of the acceptor levels due to the vacancy and introduction of impurity level. Moreover, the optical properties of ZnTe are improved as the absorption spectra show a remarkable redshift and the electron transition of the defect systems in the visible region are enhanced apparently accompanied with appearance of dielectric peaks.

Keywords: ZnTe first-principles electronic structure optical property

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