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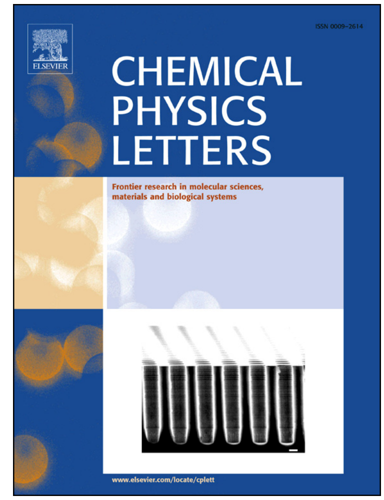

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Effect of Zr doping on the electrical and optical properties of ZnO

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Abstract

Within 0.02083-0.04167 Zr doping amount, there are contradictory reports on the experimental results of ZnO doping system in absorption spectrum distribution. However, there is no reasonable theoretical explanation until now. To solve this problem, density functional theory-based generalized gradient approximation plane wave ultra-soft pseudopotential GGA+U method is utilized in this paper and the first-principles are adopted to construct the supercell models with three different doping amounts, $Zn_{0.97917}Zr_{0.02083}O$, $Zn_{0.96875}Zr_{0.03125}O$ and $Zn_{0.95833}Zr_{0.04167}O$. On the basis of geometrical optimization of all the models, band structure distribution, density of states distribution and absorption spectrum distribution are calculated and the calculation results show that within the limited doping amount, the higher the Zr doping amount is, the higher the doping system volume is, the higher the total energy is, the lower the system stability is, the higher the formation energy is, and the more difficult doping is. With all the doping systems converted into n-type degenerate semiconductor, the wider the doping system band gap is, the more significant the absorption spectrum blueshift is, the lower the absorption intensity is, the higher the electronic effective mass is, the higher the electronic concentration is, the lower the electronic mobility is, the higher the electronic conductivity is, and the more significant the doping system conductivity is. The calculation results and the experiment results are consistent.

Keywords: Zr doping; ZnO; electrical and optical properties; first-principle calculation

1. Introduction

As a wide band gap II-VI compound semiconductor, the band gap of ZnO at 300K is 3.37eV. Compared with another widespread wide band gap GaN semiconductor, ZnO owns high exciton binding energy (60 meV). ZnO usually manifests n-type semiconductor. However, different-element doping enables ZnO to own many new functions, for example, transparent electrodes, flat-panel display, light-emitting diode, solar cell and surface acoustic wave device [1-7]. Effective element doping has a stable structure in ZnO semiconductor [8], so photoelectric properties of ZnO doping system have been a current research hotspot [9-12]. In experimental studies, studies on the photoelectric properties of Zr-doped ZnO are widespread, for example, Selvam et al. [13] adopted low-cost coprecipitation method to study the influences of Zr-doped ZnO system structure and photocatalytic performance. The results indicate that the grain size of Zr-doped ZnO is small and the surface area is high. Also within 0.2-1at% Zr-doping, the higher the doping amount is, the stronger the photocatalytic activity is. Tsay et al.,