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Electronic structure and optical property studies of wurtzite $AgInS_2$ doped by tin

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ABSTRACT

The electronic structure and optical property of wurtzite $AgInS_2$ with vacancy defects and tin doping have been investigated by the first principle based on density functional theory. The results show that the intrinsic silver and indium vacancy may lead to the narrowing of bandgap. It shows metal characteristic after a silver atom and an indium atom are respectively replaced by tin atoms in the supercell of wurtzite $AgInS_2$. The optical property study indicates that the absorption curves and reflectivity curves of $AgInS_2$ are blue shift and weakened owing to the existence of vacancy defects and tin doping.

1. Introduction

As a I–III–VI ternary metal compound, $AgInS_2$ is widely used in the fields of photovoltaic cells, photocatalysis, optoelectronics and nonlinear optics due to its excellent optical property and environmentally benign nature [1–3]. In general, $AgInS_2$ crystals have two different polymorphs: chalcopyrite phase and orthorhombic wurtzite phase. The latter has shown more excellent photoelectrical and optical property than that of chalcopyrite, and it has attracted much concentration [4,5]. The experiments and simulated calculations of pure orthorhombic wurtzite $AgInS_2$ indicated that it was a direct bandgap semiconductor with a proper range of light absorption [6,7]. Yet, due to the optical property of pure orthorhombic wurtzite $AgInS_2$ has encountered development limitations, researchers have adopted various routes to improve the property. Metal ion doping is the most effective way to improve optical property of orthorhombic wurtzite $AgInS_2$ for the introduction of impurity levels can improve the bandgap effectively, and it has been found by experiments in recent year that tin doped $AgInS_2$ has very excellent optical property due to the adjustable band gap in the visible region [8–10]. Therefore, it is necessary to study the optical principle of $AgInS_2$ doped by tin via simulated calculation, and it can also offer a valuable proposal for the experiment researchers of $AgInS_2$ study.

The first principle can be used to calculate the band gap and optical property of a semiconductor [11–13]. It has been widely used in optical material calculation to explain the results of experiment of optical materials [14,15]. Doping calculation of a semiconductor is an important application of the first principle, and it has been reported by more and more papers [16–18]. For example, Zhang and his partners calculated hydrogen absorption of the graphene oxide doped by Mg via the first principle calculation [19]; Caliskan and Guner calculated the spin dependent electronic behavior of ZnO doped by Co via the first principle study [20]; Li and his coworkers studied the energy band structure of $BiPO_4$ doped by N via the first principle [21].

In this work, the first principle is adopted to study the electronic structure and optical property of $AgInS_2$ doped by tin, and the purpose is to carry out a theory study of $AgInS_2$ with different structural defects and offer a proposal for the researchers of experiment.

2. Computational details

The first principle calculation of $AgInS_2$ was carried out with the Cambridge Serial Total Energy Package module (CASTP) of material studio 6.0 version. The calculation adopted the supercell of wurtzite $AgInS_2$, which consisted 32 atoms. The core electrons were

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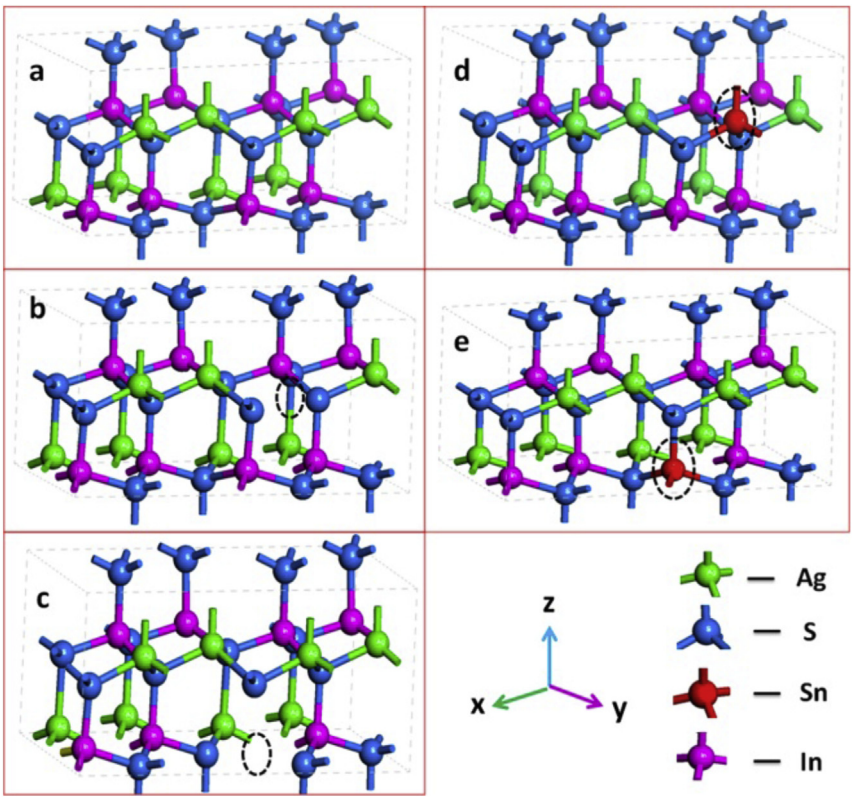

Fig. 1. The supercell crystal structure models of wurtzite $AgInS_2$ with different structural defects. (a) The supercell crystal structure models of pure wurtzite $AgInS_2$; (b) The supercell crystal structure models of wurtzite $AgInS_2$ with silver vacancy; (c) The supercell crystal structure models of wurtzite $AgInS_2$ with indium vacancy; (d) The supercell structure models of wurtzite $AgInS_2$ a silver atom of which is replaced by a tin atom; (e) The supercell structure models of wurtzite $AgInS_2$ an indium atom of which is replaced by a tin atom.

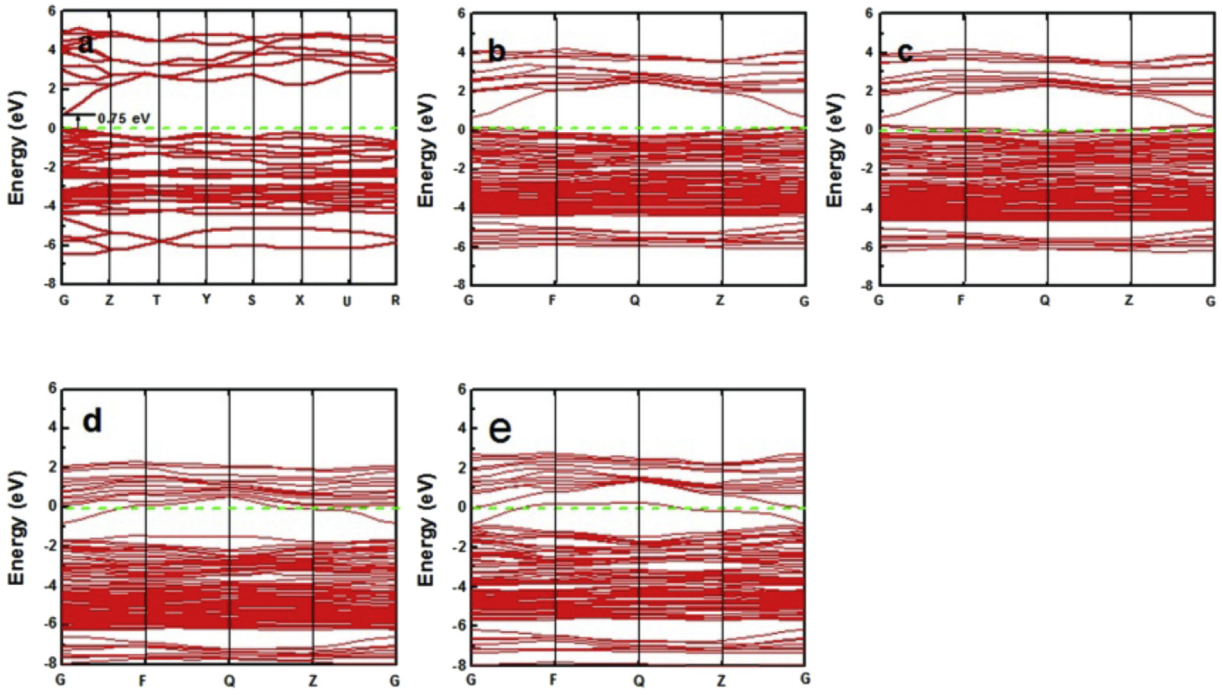

Fig. 2. Band structure of wurtzite $AgInS_2$ with different structural defects. (a) Band structure of pure wurtzite $AgInS_2$; (b) Band structure of wurtzite $AgInS_2$ with silver vacancy; (c) Band structure of wurtzite $AgInS_2$ with indium vacancy; (d) Band structure of wurtzite $AgInS_2$ a silver atom of which is replaced by a tin atom; (e) Band structure of wurtzite $AgInS_2$ an indium atom of which is replaced by a tin atom.