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半导体光电

Sb掺杂ZnO电子结构和光学性质

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摘要：

为了研究ZnO掺Sb后电子结构和光学性质的变化，采用基于密度泛函理论对纯净ZnO和Sb掺杂ZnO两种结构进行第一性原理的计算。计算结果表明：随着Sb的掺入，体系的晶格常数变大，键长增加，体积变大，系统总能增大。能带中价带和导带数目明显变密，费米能级进入导带，体系逐渐呈金属性，带隙明显展宽。在光学性质方面，主吸收峰的左边出现了新的吸收峰，是由导带上的Zn-4s和Sb-5p轨道杂化电子跃迁所致；同时介电函数虚部波峰发生一定程度的升高，实部静态介电常数也明显增大。

关键词： 材料 氧化锌 第一性原理 光学性质 掺杂

Electronic Structure and Optical Properties of Sb doped on ZnO

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Abstract:

The electronic structure and optical properties of doped Sb in ZnO, together with the corresponding results of pure ZnO for comparison, had been systematically studied from the first principles based on density functional theory. The calculated results show that for ZnO doped with Sb, the lattice constant, bond length, primitive cell volume and total energy are all larger than those of pure ZnO. For the doping case, the Fermi level becomes larger than the conduction band minimum (CBM),the system grows metallic and the band gap becomes wider. For the optical properties, a new absorption peak appear near the main peak, which is mainly attributed to the transition of orbital electrons of Zn-4s and Sb-5p. Finally, it is also pointed out that for the dielectric function, the peak values of imaginary part and the ε(0) value of real part become larger.

Keywords: materials ZnO first-principles optical properties doping

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