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论文

ZnO/GaN核壳异质结电子结构和光学特性第一性原理研究

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摘要：

采用密度泛函理论框架下的第一性原理方法计算了ZnO/GaN核壳异质结的电子结构和光学特性.计算结果表明:[10 $\bar{1}$0]和[11 $\bar{2}$0]晶面的异质结在带隙边缘价带顶和导带底的电子态密度各自主要由氮原子和锌原子贡献.以[10 $\bar{1}$0]晶面为侧面的异质结结构的介电函数虚部(ε_2)的曲线具有相似的特征,都是价带的氮原子到导带锌原子的跃迁,但峰位依赖于核层数和壳层数的不同而有所偏移.相对地,以[11 $\bar{2}$0]晶面为侧面的结构,其ε_2的曲线与[10 $\bar{1}$0]晶面的情况有着很大的差别,其出现了一个由镓原子与氮原子之间的跃迁形成的峰.因此,可以通过控制异质结的晶面来实现对其光学特性的调控.这种新型异质结将在发光器件、光电太阳能电池、生物探测等方面具有一定的应用价值.

关键词： 异质结 电子结构 光学性质 第一性原理

First-principles Study on Electronic and Optical Properties of ZnO/GaN-Core/Shell Heterostructures

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Abstract:

The electronic and optical properties of ZnO/GaN-core/shell heterostructures are studied by using the first-principles method based on density functional theory. The results show that the top of valence bands and the bottom of conduction bands for the [10 $\bar{1}$0] and [11 $\bar{2}$0] crystal plane of heterostructures are mainly contributed by the nitrogen and zinc atoms, respectively. The heterostructures with [10 $\bar{1}$0] lateral facets have the similar imaginary parts of dielectric functions (ε_2) curves, which are all electronic transitions between the states from nitrogen at valence bands and the states from zinc at conduction bands. However, the peaks of the ε_2 curves shift slightly depending on the thickness of the core and shell. In contrast, the ε_2 curve for the heterostructures with [11 $\bar{2}$0] lateral facets is significantly different from the cases with [10 $\bar{1}$0] lateral factets.There is a new peak related to the transition between the states from gallium and the states from nitrogen. Therefore, the optical properties of the ZnO/GaN-core/shell heterostructures can be tuned by controlling the lateral facets of the heterostructures.The current work is available for the applications in light emitting device,photoelectric solar cell,and biological detection.

Keywords: Heterostructure Electronic structure Optical Properties The first-principles

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