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Using Quantum Espresso to study optical properties of ZnO

This poster aims to introduce and elucidate the combined use of Density Functional Theory (DFT) and quantum mechanics for investigating the optical properties of metal-oxide semiconductors (MOS). The study of ZnO as a semiconductor experienced significant peaks in 1990 and 2010. In 2010, over 5,000 publications contained ZnO in the title, abstract, or keywords. This occurred because ZnO possesses a wide range of properties, depending on doping, including conductivity ranging from metallic to insulating, high transparency, piezoelectricity, wide bandgap semiconductivity, room temperature ferromagnetism, and significant magneto-optical, and chemical sensing effects. Due to these properties, there has been a significant increase in the number of relevant publications.

Because of the applications such as in solar cells, gas sensors, and photocatalysts, ZnO has garnered significant attention among metal oxide semiconductors (MOS). ZnO is characterized by a direct wide bandgap (~3.3 eV) and possesses a large exciton binding energy of 60 meV. These properties render it particularly intriguing as a laser material, with the potential for exciton recombination at room temperature or even higher. One of the challenges is to obtain a p-type doping for ZnO, which has been investigated by several researchers.

ZnO crystallizes in the wurtzite structure and has probably the richest variety of different nanostructures. Wurtzite structure has basic hexagonal symmetry. The two hcp lattices have the same axis \((a_{\textsubscript{3}}\text{-axis}) \) but one of them is displaced with respect to the other. The wurtzite structure may be considered as an hcp structure with a basis of two atoms. It also has uniaxial symmetry and a number of piezoelectric and pyroelectric crystals possess this structure.

Although GaN is considered the best candidate for optoelectronic devices, ZnO offers significant advantages for LEDs and LDs due to its wide and direct bandgap, as well as a high excitonic binding energy. ZnO exhibits excellent radiation resistance, making it suitable for space applications and high-energy radiation environments. Its bandgap energy can be adjusted through alloying processes, enabling its use in heterostructured LEDs and quantum well lasers. These features make ZnO a rich family of nanostructures with diverse promising applications. ZnO, a wide bandgap semiconductor, emerges as a promising candidate to replace conventional materials in various applications, including solar cells. Theoretical physics offers a powerful approach to explore these possibilities through quantum mechanical simulations, enabling the study of material behavior, such as in ZnO.

This work delves into the application of the Quantum ESPRESSO package to calculate band structures, density of states, and optical properties of ZnO. We highlight both the limitations and advancements of this package in recent years for MOS studies. The presentation will delve into the different calculations, approximations, and generalizations possible within QE, emphasizing the key distinctions between GGA and hybrid functional-based calculations. We will also discuss the theoretical, mathematical, and computational aspects of these methods, along with their operational and computational costs. The primary areas of knowledge covered in this poster include solid-state physics, quantum mechanics, and computational simulation.

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