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Surface effects on the electronic and structural properties of ZnO nanocrystals

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Abstract – Zinc Oxide nanocrystals have been investigated by *ab-initio* simulations. Saturated and unsaturated nanoparticles were studied in this work. The saturated nanocrystals allow the understanding of quantum confinement that structures in nanoscale present. The unsaturated nanocrystals showed several surface reconstructions, inserting several impurity levels in bandgap. These surface states can be spin-polarized in such a way that nanoparticles can present a magnetization even without the inclusion of magnetic impurities, as observed experimentally.

Zinc Oxide has been largely studied due its differentiated properties. This material is a wide, direct band gap semiconductor, and is a potential candidate to applications in spintronics. When nanostructures are reduced to scale of nanometers, the ratio surface:volume become larger and different phenomena from that present in crystal can arise. Recently, a lot of works in literature have reported magnetic behavior of ZnO nanostructures without magnetic impurities[1]. This turns even more interest into this material, mainly in the nanoscale. In this work, we investigate ZnO nanocrystals by performing *ab-initio* simulations using Density Functional Theory (DFT) and the Local Density Approximation (LDA). The calculations were developed with the Vienna Ab-initio Package (VASP) employing the projected augmented wave method (PAW). Both saturated and unsaturated nanocrystals were relaxed until the forces in each cartesian coordinate were less than 25 meV/Å. The two more stable structures, wurtzite and zinc blend, were considered. The nanoparticles have sizes varying from ~0.9 nm to ~1.8 nm and they can be both centered in an atom or in a bond.

As a first step, we studied saturated nanocrystals to separate the quantum confinement effects from those originated from surface defects. The first effect observed was the increase of band gap when their size is reduced. Also we could analyze the morphology and electronic structure of these particles. We then removed the hydrogens from the nanocrystal's surface. The relaxed structure showed several reconstructions, including kinks, broken bonds, changes in bond angles, zinc dimers and so on. Due the reconstructions, a lot of surface states are inserted in band gap. For some structures, they can be spin-polarized and the structure becomes magnetic.

A deep analysis of the nanocrystals presenting this kind of magnetic behavior, shows that we can not isolate only one defect, or a point defect, that is responsible for this magnetization. So, we show that delocalized, spin-polarized surface states are the responsible for the ferromagnetic response in these nanostructures [2]. In conclusion, we emphasize that a deep comprehension of what happens in the surface of ZnO nanoparticles is the key to turn possible a future application of them in electronic/magnetic devices.

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References

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