

Abstract Submitted
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Band gap engineering in ZnO nanowire based alloys JEVERSON ARANTES, CAETANO MIRANDA, GUSTAVO DALPIAN, Universidade Federal do ABC — ZnO nanowires can be manufactured through different ways, including wet chemical routes, chemical vapor deposition and other ones. A broad range of potential applications for these nanostructures have been proposed. Here, we explore the effects of alloying on ZnO based nanostructures, through First Principles Calculations within Density Functional Theory, to better understand the quantum confinement effect. A detailed ab-initio study of the energetic, electronic and structural properties of ZnO nanowires alloyed with Be, Cd, Mg and Al has been performed. The effects of isovalent impurities such as Be, Cd, Mg is mainly to tune the band gap of the wire. For small impurity concentrations, smaller than 40 %, we observe an almost linear behavior of the band gap. These impurities tend to be randomly distributed through the wire, what indicates that it should not be very difficult to grow these structures. We have also tested the effect of alloying the wire with Al donors. For this case, we observe a strong tendency for the impurities to be localized at the surface of the wire.

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