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ab initio studie of the effect of dopant scandium on mechanical and electronic properties of zinc oxide

Zinc oxide has attracted great interest in the last few years. This is because electronics based on ZnO have wide applications and better performance on account of improved electronic conductivity, lower power consumption, better stability, fast electron transfer kinetics and improved storage capacity. ZnO crystals are able to withstand much higher electric fields than silicon crystals, such that electronic devices based on ZnO will be able to operate on higher power and higher temperature. The main drive globally is to come up with a cheap and reliable photovoltaic source. ZnO is one of the materials that can be investigated to come up with such materials. Electrical conductivity of ZnO is enhanced by doping with other suitable elements. The effect of doping indium, aluminium, yttrium and gallium in ZnO has been frequently reported by various groups but effect of rare earth metals such as scandium has scarcely been reported. The objective of this research is to study the mechanical and electronic properties of dopant Sc on ZnO using ab initio study. The main method is based on using quantum espresso code and interactive solution of the Kohn Sham equation of density functional theory in a plane wave set. From the data obtained, the band gap reduced after doping ZnO with scandium. This will therefore make the final product a highly conductive and transparent film that can be used in solar cells

Keywords

scandium,doping,zincoxide

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