

2nd World Congress and Expo on
Nanotechnology and Material Science
April 04-06, 2016 at Dubai, UAE

Ab-initio study of magnetic and optoelectronic properties of Na-doped ZnO

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We used an ab-initio calculation with FP-LAPW method and LSDA approach, we have performed a p-type Na-doped ZnO using a wurtzite structure to understand the optoelectronic and magnetic effect of $Zn_{1-x}Na_xO$ ($x=0.0625, 0.125$), the lattice parameter increased by doping with Na atoms, therefore the optical properties such as the dielectric function, the refractive index and the absorption coefficient increased and shifted to the lower energy and that was caused by the Na concentration, this result allows a good conception of the electronic devices.