Abstract

The effect of hydrogen adsorption on the electronic structures and optical properties of undoped and Mg-doped ZnO $000\bar{1}$ polar surface was investigated using the first principles method. The obtained results show that hydrogen adsorption is more favored on Mg doped-ZnO $000\bar{1}$ surface than onto the clean surface, and this makes Mg-doped ZnO and $Mg_xZn_{1-x}O$ more efficient for H storage or gas sensing applications than undoped ZnO. On the other hand, our results show that the hydrogen adsorption on the Mg doped surface is energetically very preferable when the surface was prepared under O-rich conditions. We have also examined the effect of H adsorption on the optical properties of the surface