Abstract

The effect of hydrogen adsorption on the electronic structure and properties of clean and Cu-doped ZnO$(10\bar{1}0)$ non polar surface was investigated using the first principles method. We found that the Cu-doped surface is more stable than the undoped one, and that high Cu solubility can be achieved in ZnO under O-rich condition with the use of metallic Cu as a Cu doping source. On the other hand, the obtained results show that hydrogen adsorption is more favored on Cu-doped-ZnO$(10\bar{1}0)$ surface than onto the clean surface, and this make Cu-doped ZnO surface and nanostructures more efficient for atomic H sensing applications than clean ZnO surface. We have also examined the effect of H adsorption on the surface work function of both clean and Cu-doped surfaces. We found that the adsorption of hydrogen molecule increases the work function of both surfaces, while, the adsorption of atomic hydrogen decreases significantly the surface work function