Abstract

The effect of hydrogen adsorption on the electronic structure and properties of clean and Be-doped ZnO(0 0 0 $\bar{1}$) polar surface was investigated using the first principles method. We found that the Be-doped surface is more stable than the undoped one, and that high Be solubility can be achieved in ZnO under O-rich condition with the use of metallic Be as a Be doping source. On the other hand, the obtained results show that hydrogen adsorption is more favored on Be-doped- ZnO(0 0 0 $\bar{1}$) surface than onto the clean surface, and this make Be-doped ZnO and BexZn1-xO more efficient for H gas sensing applications than clean ZnO surface. Our results show also that the Be-doped surface is more efficient for hydrogen storage applications than the clean surface. We have also examined the effect of H adsorption on the surface work function of both clean and Be-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