Abstract

In this study, the GGA-PBE method was used to study the structural and electronic properties of the $ZnAl_2O_4$(111) surface with and without oxygen vacancies. The $ZnAl_2O_4$(111) surface has six possible surface terminations called Zn(O_2), Zn(Al), Al(Zn), Al(O_2), O_2(Zn), and O_2(Al). The results obtained in this work show that the surface energy, electronic structure and work function of the $ZnAl_2O_4$(111) surface depend greatly on the nature of atoms in the top surface layer. The calculated surface energies indicate that the Zn(O_2) termination is the most stable surface termination in O-rich and Al-poor environments, while the Al(Zn) termination is the most stable termination in Al-rich and O-poor environments. On the other hand, our results show that the formation of oxygen vacancies can greatly affect the stability of the $ZnAl_2O_4$(111) surface. We found that the O-deficient surface is more stable than the perfect surface in the case of O_2(Zn) and O_2(Al) surface terminations. In the case of other surface termination, the formation energy of V_O is positive under both O-rich and O-poor conditions except the case of the Zn(O_2) termination under O-poor and Al-rich conditions. Moreover, we found that the formation of oxygen vacancies can greatly affect the stability, electronic structure, and work function of the $ZnAl_2O_4$(111) surface.