Ab-Initio Study of the Structural and Electronic Properties of Zr Adsorption on AlN (0001) Surface

W. López-Pérez,1 R. González-Hernández,1 J. Rivera-Julio,1 G. E. Escorcia-Salas,2 and J. Sierra-Ortega2

1Grupo de Física Aplicada, Departamento de Física, Universidad del Norte, Barranquilla, Colombia.
2Grupo de Investigación en Teoría de la Materia Condensada, Universidad del Magdalena, Santa Marta, Colombia.

We have performed spin-polarized first-principles calculations to explore the Zr adsorption and diffusion on the AlN(0001)-(2×2) surface. The calculations were performed using the generalized gradient approximation (GGA) [1] with ultrasoft pseudopotential [2] within the density functional theory (DFT) [3]. We found that the most energetically favorable structure corresponds to the Zr-T4 reconstruction or the Zr adatom located at the hcp-hollow (T4) site, while the Zr adsorption on-top of an aluminium atom (T1 position) is energetically unfavorable. The Zr diffusion on surface shows an activation energy of 0.473 eV (T4 to H3). The resultant reconstruction of the Zr adsorption on AlN(0001)-2×2 surface presents a lateral relaxation of some hundredth of Å in the most stable site. The comparison between the electronic structure of the AlN(0001) clean-surface and with Zr adatom is also examined. The clean surface aluminium-terminated has one Al dangling-bond in the top layer. We found that the clean AlN(0001) surface layer have metallic behavior, due to the partial occupation of the Al dangling-bond band by 0.75 of an electron, disappearing the existing gap in the bulk AlN. The existence of a partially filled state means that this state gives rise to a metallic surface with the Fermi energy crossing the surface state. The Zr adsorption saturates some dangling bonds of the clean surface and the system presents a metallic behavior in both spin components.

This work is funded by the División de Investigación, Desarrollo e Innovación, Universidad del Norte, Barranquilla, Colombia.


Contact: wlopez@uninorte.edu.co