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

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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-T_4 reconstruction or the Zr adatom located at the hcp-hollow (T_4) site, while the Zr adsorption on-top of a aluminium atom (T_1 position) is energetically unfavorable. The Zr diffusion on surface shows an activation energy of 0.473 eV (T_4 to H_3). The resultant reconstruction of the Zr adsorption on AlN(0001)-2×2 surface presents a lateral relaxation of some hundredth of Åin 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.

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[1] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. B **77**, 3865 (1996).

[2] D. Vanderbilt, Phys. Rev. B **41**, 7892 (1990).

[3] P. Hohenberg and W. Kohn, Phys. Rev. **136**, 864 (1964).

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