XIV International Congress of the Mexican Hydrogen Society
Cancun, Mexico, 2014

A DFT Study of O_2 Adsorption on Periodic $Ga_{1-x}N_x$ (100) Surface

L.C. de la Portilla-Maldonado[1], R. Mendoza-Pérez[2], G. Contreras-Puente[3], F de L. Castillo-Alvarado[3], A. Cruz-Torres[3,*], M. López-López[4]

[1]Departamento de Ciencias Básicas, División de Ciencias Básicas e Ingeniería, Universidad Autónoma Metropolitana-Azcapotzalco, Av. San Pablo 180 Col Reynosa Tamps, Azcapotzalco, 02200, México D. F.,

[2]Universidad Autónoma de la Ciudad de México; Av. Prolongación San Isidro 151; Col. San Lorenzo Tezonco; C. P. 09790; México, D. F.

[3]Escuela Superior de Física y Matemáticas. IPN, Edificio 9 U: P: Adolfo López Mateos, Col. San Pedro Zacatenco. Del. Gustavo A. Madero, 07738, México D. F.

[4]Departamento de Física, Centro de Investigación y Estudios Avanzados del IPN, México DF.

[*]Tel: 5563667484; e-mail: acruztorres@yahoo.com.mx

ABSTRACT

The adsorption of molecular oxygen on $Ga_{1-x}N_x$ (100) surface has been explored. This work was achieved using Accelrys Material Studio software for material modeling and simulation applying CASTEP library. With that kind of library it was obtained the geometry optimization. Moreover, this job is done by density functional theory (DFT) model using generalized gradient approximations (GGA) an enhanced with 1996 gradient-corrected correlation functional of Perdew, Burke and Ernzerhof. With this software we also calculated the density of states, the number of electrons, up and down number of spins, chemisorption and repulsion energies for O_2 on $Ga_{1-x}N_x$ (100), etc. We compare our results with theoretical and experimental data obtained in the literature.

Keywords: Electronic band stucture; Ab initio calculations; Nitrides