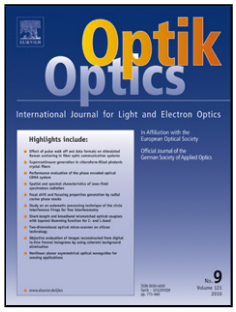

Title: Theoretical study on the electron structure and optical properties of Cs adsorption on $In_{0.53}Ga_{0.47}As$ (100) β_2 (2×4) reconstruction surface

Author: Lin Yin Liang Chen Shuqin Zhang Minyou He Lingai Su Yunshen Qian

PII: S0030-4026(16)31274-8
DOI: http://dx.doi.org/doi:10.1016/j.ijleo.2016.10.107
Reference: IJLEO 58379

To appear in:

Received date: 26-8-2016
Accepted date: 25-10-2016

Please cite this article as: Lin Yin, Liang Chen, Shuqin Zhang, Minyou He, Lingai Su, Yunshen Qian, Theoretical study on the electron structure and optical properties of Cs adsorption on In0.53Ga0.47As (100) β2 (2×4) reconstruction surface, Optik - International Journal for Light and Electron Optics http://dx.doi.org/10.1016/j.ijleo.2016.10.107

Theoretical study on the electron structure and optical properties of Cs adsorption on $In_{0.53}Ga_{0.47}As$ (100) β_2 (2×4) reconstruction surface

Lin Yin[a] , Liang Chen[a,b,*] , Shuqin Zhang[a] , Minyou He[a] , Lingai Su[a] , Yunshen Qian[b]

[a] *Institute of Optoelectronics Technology, China Jiliang University, 310018 Hangzhou, China*

[b] *Institute of Electronics Engineering & Optoelectronics thchnology, Nanjing University of Science and Technology, 210094 Nanjing, China*

ABSTRACT

Cs activation on $In_{0.53}Ga_{0.47}As$ (100) β_2 (2×4) reconstruction surface is an important process for improving the performance of the negative electron affinity (NEA) photocathode. Using the first-principles method based on the density functional theory (DFT), within scope of the generalized gradient approximation (GGA), the electronic structure and optical properties of Cs adsorption on $In_{0.53}Ga_{0.47}As$ (100) β_2 (2×4) reconstruction surface models are calculated and analyzed in this article. The results show that adsorption energy is negative suggesting that the structure of Cs adsorption on $In_{0.53}Ga_{0.47}As$ (100) β_2 (2×4) surface is stable. The Cs adsorption on $In_{0.53}Ga_{0.47}As$ (100) β_2 (2×4) surface makes work function lower and energy band bend, which is benefit for electrons escape to the surface. At the same time, new energy bands are generated. Combined with study of the $Al_{0.5}Ga_{0.5}As$ (100) β_2 (2×4) reconstructed surface, two different elements of Al and In are compared under the Cs atomic adsorption. The work function and band gap of Cs atom adsorption on In atom are all smaller than adsorption on Al atom. And the absorption coefficient, dielectric function and energy loss function of Cs adsorption on $In_{0.53}Ga_{0.47}As$ (100) β_2 (2×4) surface and clean $In_{0.53}Ga_{0.47}As$ (100) β_2 (2×4) surface are researched and compared. Cs adsorption on surface makes the peaks of absorption coefficient, dielectric function and energy loss function of surface higher than that of clean $In_{0.53}Ga_{0.47}As$ (100) β_2 (2×4) surface. The analysis is helpful to further strengthen the study for near-infrared material photoemission.