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# Theoretical study on the electron structure and optical properties of Cs adsorption on $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ (100) $\beta_2$ (2×4) reconstruction surface

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## ABSTRACT

Cs activation on  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  (100)  $\beta_2$  (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  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  (100)  $\beta_2$  (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  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  (100)  $\beta_2$  (2×4) surface is stable. The Cs adsorption on  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  (100)  $\beta_2$  (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  $\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}$  (100)  $\beta_2$  (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  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  (100)  $\beta_2$  (2×4) surface and clean  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  (100)  $\beta_2$  (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  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  (100)  $\beta_2$  (2×4) surface. The analysis is helpful to further strengthen the study for near-infrared material photoemission.

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