

Tuning the electronic and magnetic properties of 2D g-GaN by H adsorption: An ab-initio study

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Abstract

We have theoretically studied the structural, electronic and magnetic properties of the hydrogen adsorption on a honeycomb gallium-nitride two-dimensional monolayer (2D g-GaN). Results indicate that the band gap energy can be systematically tuned by the hydrogen coverage on the 2D g-GaN in the diluted limit. In addition, a total magnetic moment can be induced in the 2D g-GaN by hydrogen adsorption due to s-p interaction and band structure effects. Although hydrogen adsorption on top of nitrogen atoms shows the most stable energy in the 2D g-GaN, the most stable ferromagnetism -with a nonzero magnetic moment-is obtained when hydrogen is adsorbed on top of Ga atoms. These results indicate that H adatoms on the 2D g-GaN systems could be a potential candidate for future spintronic applications.

Keywords: