First-principles study of Ga-N co-doped graphene nanostructures

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Graphene's physical properties have made it interesting and used in a range of fields of science and technology, such as medicine, nanoelectronics, sensors, and desalination. A simple method for manufacturing graphene with scotch tape was discovered in 2004. Graphene is a two-dimensional material, one carbon atom thick. The structure of graphene is provided as a hexagonal lattice, where the carbon atoms are linked by sp^2 bonds.

Graphene would be a good material for sensors. Single molecules of a chemical can be easily detected by using sensitive sensors. Graphene has the advantages of large surface area, high chemical and thermal stability. However, pristine graphene does not have excellent ability to detect gas molecules.

It is well known that the modification of graphene with various elements leads to a change in its chemical activity.

Based on this, in our work, a modification of graphene is provided by replacing carbon atoms with gallium and nitrogen atoms in order to change the chemical activity.

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