Abstract

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Detection of chemical species in environment or gas leak in hazardous work is of a great concern as it involves health, safety and environmental risks. In an attempt to improve gas sensing performance, nanomaterials are being considered as a promising tool to overcome the main limiting factor of gas sensor technology; selectivity and sensitivity, response time and stability. Recent advances in the fabrication of silicene devices have raised exciting prospects for practical applications such as gas sensing. We investigated the gas detection performance of silicene nanosensors for four different gases (NO, NO_2, NH_3 and CO) in terms of sensitivity and selectivity, employing density functional theory and non-equilibrium Green's function method. The structural congurations, adsorption sites, binding energies and charge transfer of all studied gas molecules on silicene nanosensors are systematically discussed in this work. Our results indicate that pristine silicene exhibits strong sensitivity for NO and NO_2, while it appears incapable of sensing CO and NH3. In an attempt to overcome sensitivity limitations due to weak van der Waals interaction of those latter gas molecules on the device, we doped pristine silicene with either B or N atoms, leading to enhanced binding energy as well as charge transfer, and subsequently a signicant improvement of sensitivity. A distinction between the four studied gases based on the silicene devices appear possible, and thus promising to be next-generation nanosensors for highly sensitive and selective gas detection.

Keywords : Silicene, Nanodevices, Density Functional Theory, Gas sensor