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Highly Sensitive and Selective Gas Detection Based on Silicene

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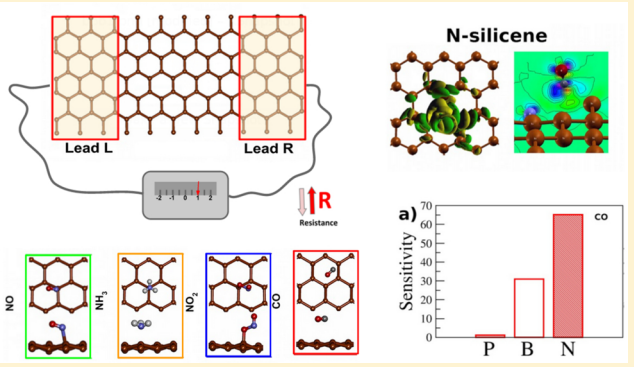
Supporting Information

ABSTRACT: 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 nonequilibrium Green's function method. The structural configurations, 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 NH_3. 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 significant improvement of sensitivity. A distinction between the four studied gases based on the silicene devices appears possible, and thus these promise to be next-generation nanosensors for highly sensitive and selective gas detection.



INTRODUCTION

Two-dimensional nanostructure materials have taken the front row in innovative applications in the past decade after the successful experimental exfoliation of graphene. Gas sensors based on graphene have attracted much attention since graphene has excellent sensitivity to detect various gas molecules, large sensing area per unit volume, low electronic temperature noise, fast response time, and high chemical stability.[1,2] The potential use of graphene for gas detection has been intensively investigated both experimentally[3−5] and theoretically.[6−8] However, growth of graphene over large surface areas is constrained. This motivated the search for other materials with similar favorable properties. In turn, this has led to the discovery of silicene as a silicon counterpart. The good properties with versatile silicon based nanotechnology gives the edge to silicene rather than graphene. This serves as the motivation of our work to theoretically explore the applicability of silicene for gas sensing.

The massless Dirac Fermions are the main reasons behind the ultrahigh carrier mobility for both the honeycomb structures of silicene and graphene.[9,10] Geometrically, the hexagonal structure of silicene has a larger size due to the larger ionic radius of Si atoms,[11] but they have similar electronic structures. One important demarcation between the two structures is a buckled formation in silicene. This is due to sp^3 and sp^2 hybridization[12] rather than only sp^2 hybridization. This feature leads to a few prominent differences in the properties of silicene and graphene. Band gap tuning with an external electric field[13,14] and with the binding adsorbates[15−17] can be seen more profoundly in silicene than in graphene.[18,19] Although free-standing silicene has not been achieved so far, recent progress shows that it can be synthesized experimentally by depositing silicon on different surfaces such as silver,[20,21] gold,[22] zirconium diboride,[23] and iridium.[24]

To date, a wide range of potential applications of silicene have been proposed in various field such as spintronics,[25,26] FETs,[27−30] hydrogen storage,[31,32] and sensing devices.[33,34] Nevertheless, using silicene as gas sensor has not been given the

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