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Title: Highly Sensitive Graphene Antidot Lattice Chemiresitor Sensor

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## Abstract

The high carrier mobility of graphene allows a short response time needed in environmental and biomedical sensing applications. In addition, the excellent mechanical properties of graphene render it for facile fabrication of sensors. Recently, many theoretical and experimental studies have been conducted on graphene-based chemical sensors. However, the conductance of semi-metallic graphene can only be weakly modulated. Therefore, the sensitivity of pristine graphene chemiresistors, as a kind of chemical sensors, was reported to be very low because conducting paths exist around the adsorbed molecules, which reduce the sensitivity. In contrast, defective graphene shows a relatively large sensitivity, where not many conducting paths exist around the defects and therefore adsorbed molecules can modulate the conductance significantly [1]. In this work we suggest a new graphene-based structure, known as graphene antidot lattice [2], for chemiresistor devices. By introducing regular antidots in a graphene sheet, a direct bandgap semiconductor material can be achieved [3]. Therefore, this structure allows for a better controllable of the electrical properties. Besides a high boundary-edge to area ratio, in graphene antidot lattices dangling bonds are chemically activated and they can adsorb different gas molecules, which can strongly affect the electronic bandstructure. Using firstprinciple calculations, we evaluate the bandstructure modifications in the presence of one and two NH3 molecules at the edge of antidots. Using the extracted transmission function, the current-voltage characteristic is obtained employing the Landauer formula. The significant change in the bandgap results in a highly sensitive chemiresitor. This result can be used to develop faster and more sensitive graphene-based chemical sensors.

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