# Supporting Information

## Ultra-sensitive NO gas sensor based on the graphene oxide coated long period fiber grating

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Support:

A total of $5 \times 5$ graphene unit cell (containing 50 carbon atoms, GP) was used as the substrate. Compared with the unit cells of $4 \times 4$ [1] and $3\sqrt{3} \times 5$ [2] in the previous literature, it should be large amplitude for the reaction $NO + \frac{1}{2}O^2 \rightarrow NO^2$. In order to minish the interaction between different layers of graphene [3], the vacuum degree in the vertical direction of graphene is set as 20 Å. Although we can confirm that the oxygen functional groups on GO surface mainly exist in the form of hydroxyl and epoxy groups through previous studies [2], the exact atomic structure of GO is still uncertain. Therefore, the model was designed following the GO model of Tang and CaO [1], and graphene oxides (GOs) were prepared by graphene substrate grown with single hydroxyl and epoxy groups. All calculations were based on the density functional theory (DFT). A plane-wave basis set with cut-off energy 350 eV was employed. [4] The Brillouin zone was sampled with a $5 \times 5 \times 1$ k-points. The calculated bond lengths of N-O in isolated nitric oxide molecule and C-C in GO are 1.151 and 1.42 Å, respectively, which are corresponding with published papers [5]. The adsorption energy ($E_{ads}$) is defined as:

$$E^{ads} = E^{tot} - (E^{mol} + E^{sheet}) \qquad \text{Eq. (1)}$$

where $E_{tot}$, $E_{mol}$, and $E_{sheet}$ represent the energies of total model, the isolated NO molecule and the GO sheet, respectively.

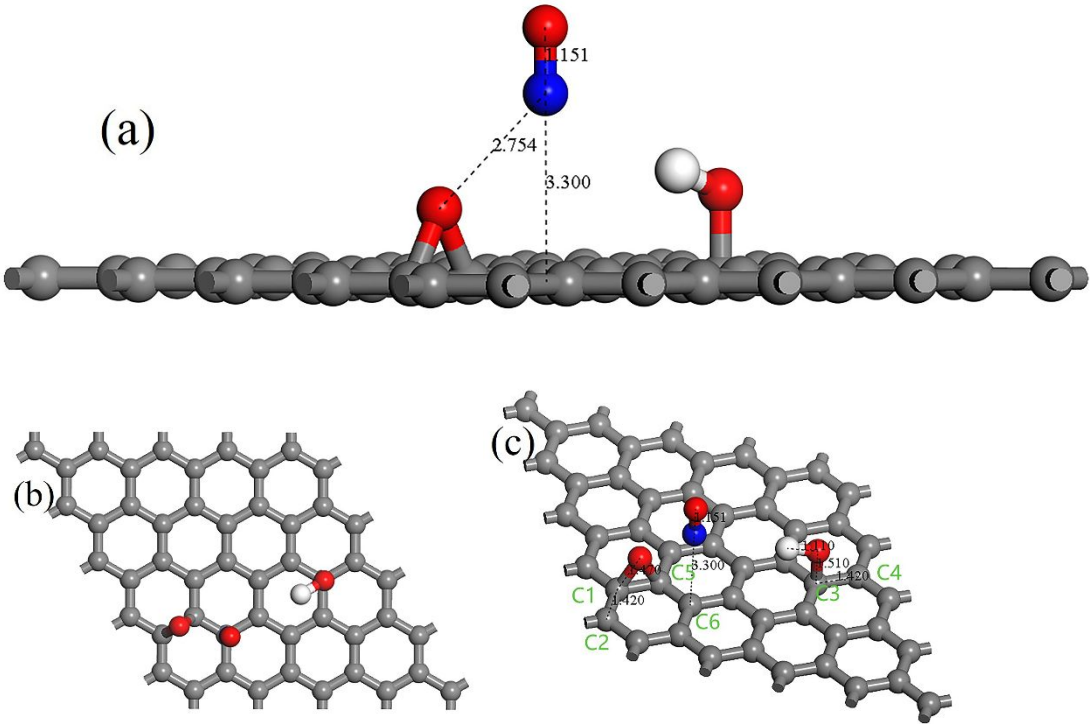


Fig. S1. The initial structures of HO-OGP. White, red, gray and blue spheres denote H, O, C and N atoms, respectively. (a) side observation; (b) top observation; (c) 45° tilt observation. All lengths are given in Å.

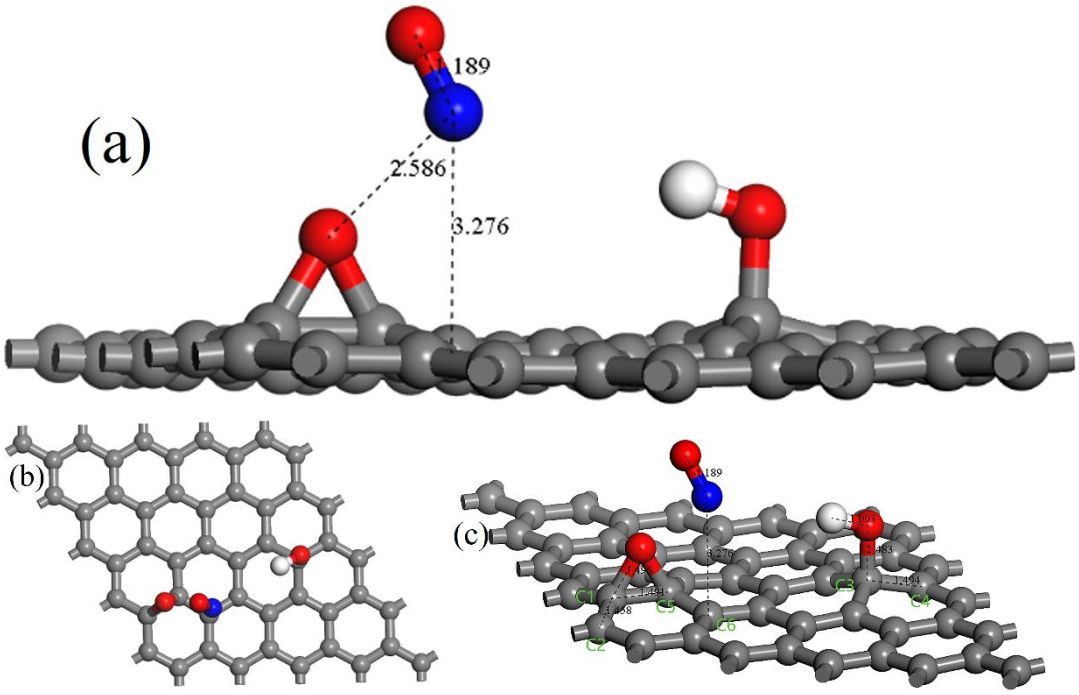


Fig. S2. The final structures of HO-OGP. White, red, gray and blue spheres denote H, O, C and N atoms, respectively. (a) side observation; (b) top observation; (c) 45° tilt observation. All lengths are given in Å.

**References**

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[2] Tang S, Cao Z. Adsorption of Nitrogen Oxides on Graphene and Graphene Oxides: Insights from Density Functional Calculations. Journal of Chemical Physics, 2011, 134(4):044710.

[3] Yang M, Zhou M, Zhang A, et al. Graphene Oxide: An Ideal Support for Gold Nanocatalysts. Journal of Physical Chemistry C, 2012, 116(42):22336–22340.

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