



## Supporting Information

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Experimental Sensing and Density Functional Theory Study of  
H<sub>2</sub>S and SOF<sub>2</sub> Adsorption on Au-Modified Graphene

*Xiaoxing Zhang,\* Lei Yu, Xiaoqing Wu, and Weihua Hu*

## SUPPORTING INFORMATION

In order to find out the most stable and possible position that Au atom forms on the graphene surface, the formation energy, which is short for  $E_{form}(C \rightarrow Au)$ , of every modification model was calculated in DFT study. The  $E_{form}(C \rightarrow Au)$  was calculated through the principle formula:

$$E_{form}(C \rightarrow Au) = E_{tot}(Au - functionalized) - E_{tot}(pristine) + \mu_C - \mu_{Au} \quad (S.1)$$

where  $E_{tot}(Au-functionalized)$  represents for the total energy of Au modified graphene;  $E_{tot}(pristine)$  represents for the total energy of pure graphene;  $\mu_C$  and  $\mu_{Au}$  are the energy of single atom in individual crystal.

Table S1 gives out the formation energies of H, B and T site models. The T site model is proved to be with the lowest energy, indicating that the T site model is the most possible position for Au.

Table S1 Formation energy of Au-modified graphene			
Position	H site	B site	T site
$E_{form}(C \rightarrow Au)$ (eV)	1.71	1.42	0.89