Electronic Supplementary Information

A density functional theory study on the adsorption of different organic sulfides on boron nitride nanosheet

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Table S1. DFT calculated adsorption energy (E_{ad}) of methanethiol (**MT**) on the model BN ($B_{27}N_{27}H_{18}$) nanosheet with different levels of basis set, solvents, methods and at different adsorption sites.*

B3LYP-D3BJ	E_{ad} (kcal/mol)
6-31G(d,p) (site 1,default)**	-5.8
6-311G(d,p)	-5.1
6-31G(d,p), n-heptane	-5.2
6-31G(d,p), n-dodecane	-5.3
6-31G(d,p), site 2**	-5.7
6-31G(d,p), site 3***	-6.1

*The exchange and correlation functional used is GD3BJ corrected B3LYP. The adsorption energy (E_{ad}) was calculated by $E_{ad} = E_{sulfur/BN} - E_{BN} - E_{sulfur} + E_{BSSE}$. See the computational details in the main text as well.

** Schematic diagram of different adsorption sites can be seen in Figure S1. The optimized geometries of MT adsorption on site 2 and site 3 can be seen in Figures S1b, and S1c, respectively. Optimized geometry of MT adsorption on site 1 can be seen in Figure 2a in the main text.

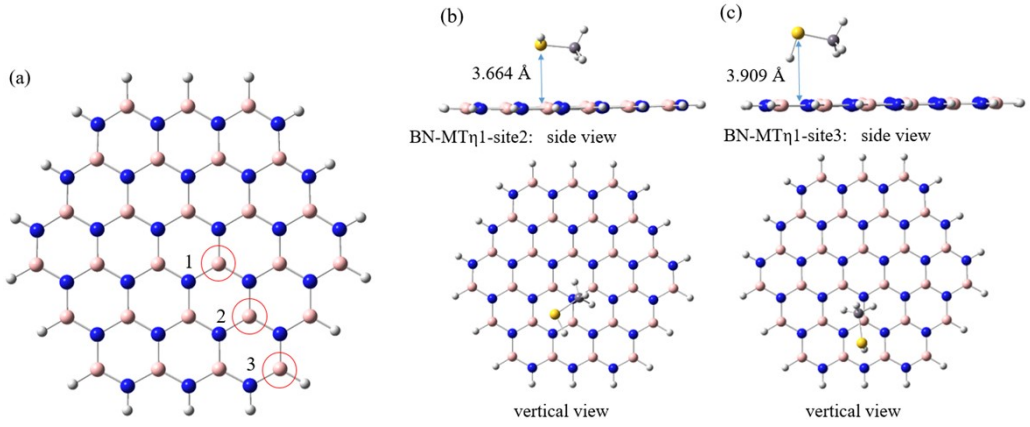

Figure S1. (a) Schematic diagram of methanethiol (**MT**) adsorption at three different sites on the model BN monolayer. (b) Optimized geometries of methanethiol (**MT**) adsorbed on the h-BN monolayer at site 2 with side and vertical views. (c) Same as (b) with the difference in the adsorption site of site 3. Adsorption configuration: $\eta 1$. The results about the case of site 1 are reported in the main text.

**** Interestingly, although the adsorption conformation of **MT** has a moderate change, the adsorption energy does not have a noticeable change (see entries #1, 5, 6 for comparison). This may be due to that the adsorption driven force is primarily composed of electrostatic and vdw interactions. Since the adsorption energies on these sites are close, and site 1 as well as the central BN ring shown in Figure S1a best represents the adsorption site(s) on BN sheet or plane in general, the adsorption behavior sulfur compounds on the central BN ring in the BN sheet was studied in this work.

Table S2. DFT calculated adsorption energy (E_{ad}) of methanethiol (**MT**) on the a B_3N_3 ring with different levels of basis set and computational method.*

Computational method/ basis set level	E_{ad} (kcal/mol)** With zero-point energy correction
B3LYP-D3BJ/6-31G(d,p)	-23.7
B3LYP-D3BJ/6-311G(d,p)	-23.3
B3LYP-D3BJ/6-311++G(d,p)	-24.3
M06-2X-D3/6-31G(d,p)	-22.6
M06-2X-D3/6-311G(d,p)	-22.8
M06-2X-D3/6-311++G(d,p)	-23.6
MP2/AGU-CC-PVDZ	-22.9

* The adsorption process can be expressed as:

MT + B_3N_3 = MT-B_3N_3 (adsorbed on B end).

** The adsorption energy (E_{ad}) was calculated by $E_{ad} = E_{sulfur/BN} - E_{BN} - E_{sulfur} + E_{BSSE}$. See the computational details in the main text as well.