Supporting Information

Engineering of the interactions of volatile organic compounds with MoS_2

Xiao-Qing Tian[a], Lin Liu[a], Xiang-Rong Wang[b, c], Ya-Dong Wei*[a], Juan Gu[a], Yu Du*[a], and Boris I. Yakobson[d].

[a]*College of Physics and Energy, Shenzhen University, Shenzhen 518060, Guangdong, P. R. China.*

[b]*Department of Physics, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong.*
[c]*HKUST Shenzhen Research Institute, Shenzhen 518057, China.*
[d]*Department of Materials Science and NanoEngineering, Department of Chemistry, and the Smalley Institute for Nanoscale Science and Technology, Rice University, Houston, Texas 77005, United States.*

1. Three configurations of VOCs adsorption on pristine MoS_2 substrates.

In this paper, the most stable one among the three adsorption configurations can be determined through the calculations and comparison. Three configurations are considered for VOCs on MoS_2 substrates as shown in Fig. 1.

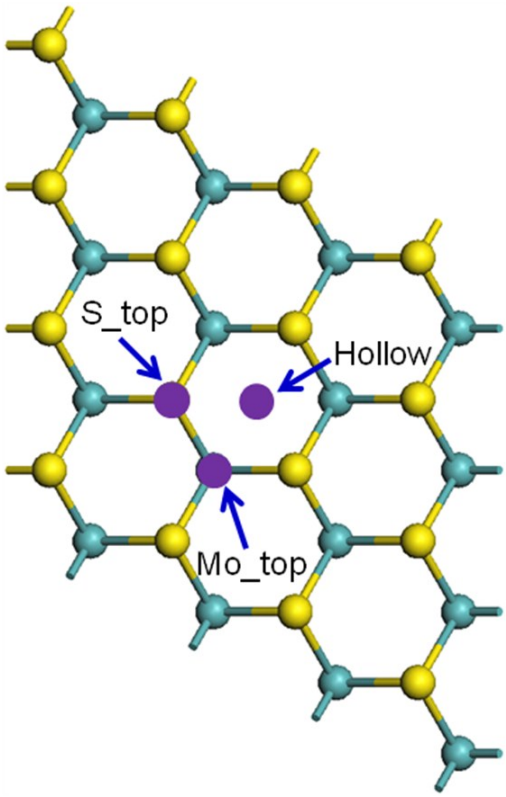

Figure 1. Top views of the functional groups of VOCs adsorption on three high-symmetry sites of MoS_2 substrates.

The adsorption energies are shown in Table S1. For ethanol molecule, the adsorption energy of Mo_top configuration is the largest. For acetone molecule, the adsorption energy of hollow configuration is the largest. For propanal molecule, the adsorption energy of Mo_top configuration is the largest. The optimized most configurations for VOCs adosortption on MoS_2 substrates are shown in Fig. 1.

Table S1. Adsorption energies of volatile organic compounds adsorbed on pristine MoS_2.

	S_top	**Mo_top**	**Hollow**
Ethanol	0.18	0.21	0.19
Acetone	0.11	0.13	0.14
Propanal	0.17	0.21	0.19

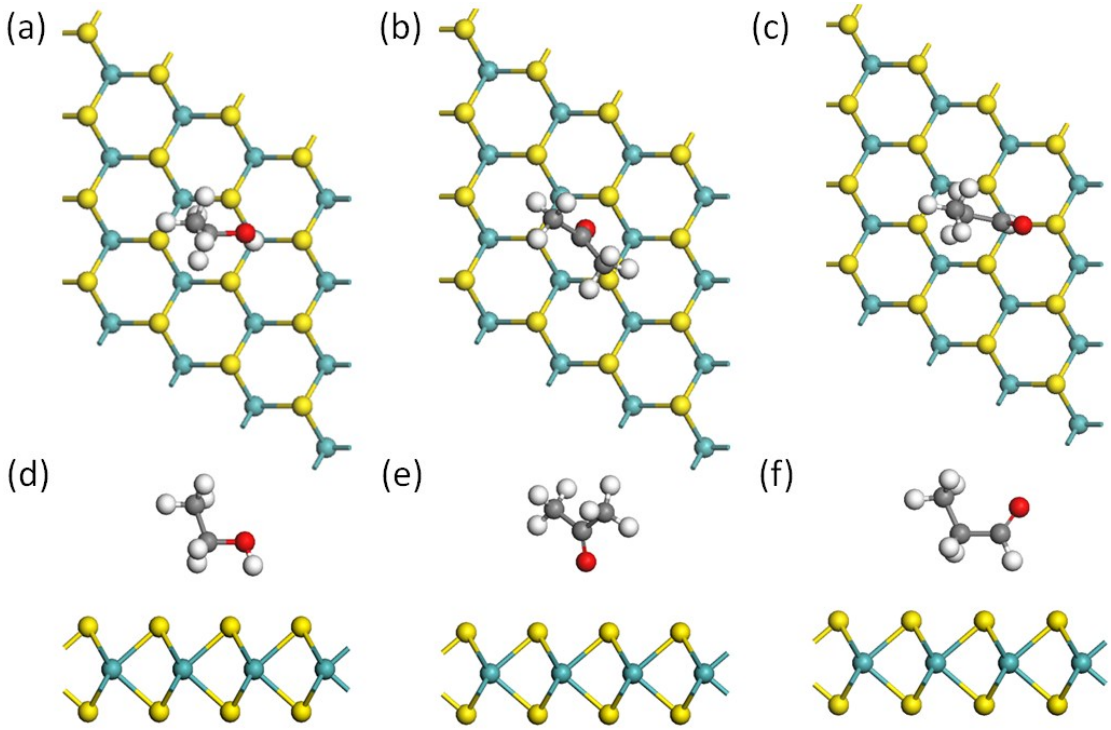

Figure S1. Top views of optimized most stable configurations of VOCs on pristine MoS_2 4×4 substrate: (a) ethanol, (b) acetone, and (c) propanal; side views of VOCs on pristine MoS2 substrate: (d) ethanol, (e) acetone, and (f) propanal. S atoms are yellow; Mo atoms are aquamarine; O atoms are red; H atoms are white; C atoms are gray. Unless stated otherwise, the results shown above were calculated by DFT-D3. Both these two notions were used through this paper.

2. Three configurations of Transition Metals (TMs) dimmers doped MoS_2 substrates.

For the transition metals (Fe, Co, Pd) doped MoS_2 substrates, three configurations are considered as shown in Fig. S2. For all TMs doped MoS_2 substrates, the dimmer1 the most stable. Set the total energy of dimmer1 as zero, the relative energies of other configurations are shown in Table S2. The energy difference of Fe doped MoS_2 substrates among different configurations is

the largest. The energy difference of Pd doped MoS_2 substrates among different configurations is the smallest.

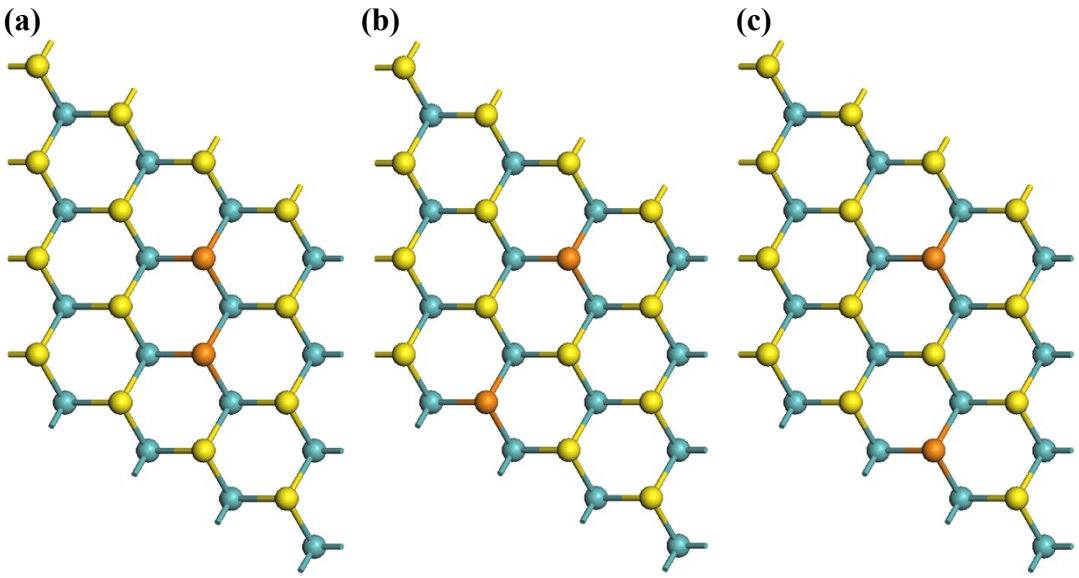

Figure S2. Top views three configurations of TM doped MoS_2 substrates: (a) dimmer1; (b) dimmer2; (c) dimmer3.

Table S2. Comparison of total energies of three configurations of TMs doped MoS_2 substrates.

	Dimmer1	**Dimmer2**	**Dimmer3**
Fe	0	1.34	1.37
Co	0	0.77	0.83
Pd	0	0.51	0.43