Supporting Information (SI):

Mechanistic insights into different types of typical VOC adsorption on monolayer MoS_2 via first-principles approaches

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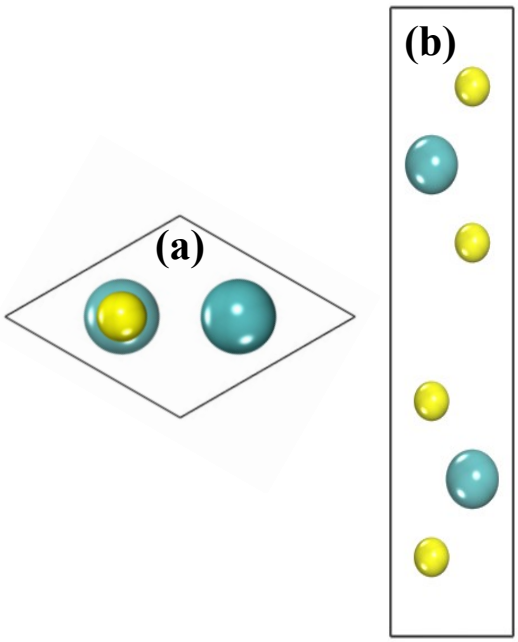

Fig. S1. Top (a) and side (b) view of the optimized bulk geometries of 2H MoS_2.

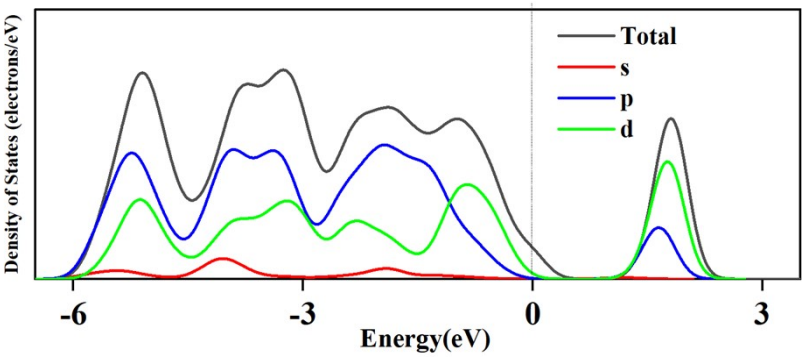

Fig. S2. The total (Total, black curve) and the projected density of states (PDOSs) of the pristine monolayer MoS_2. The Fermi level is set to zero.

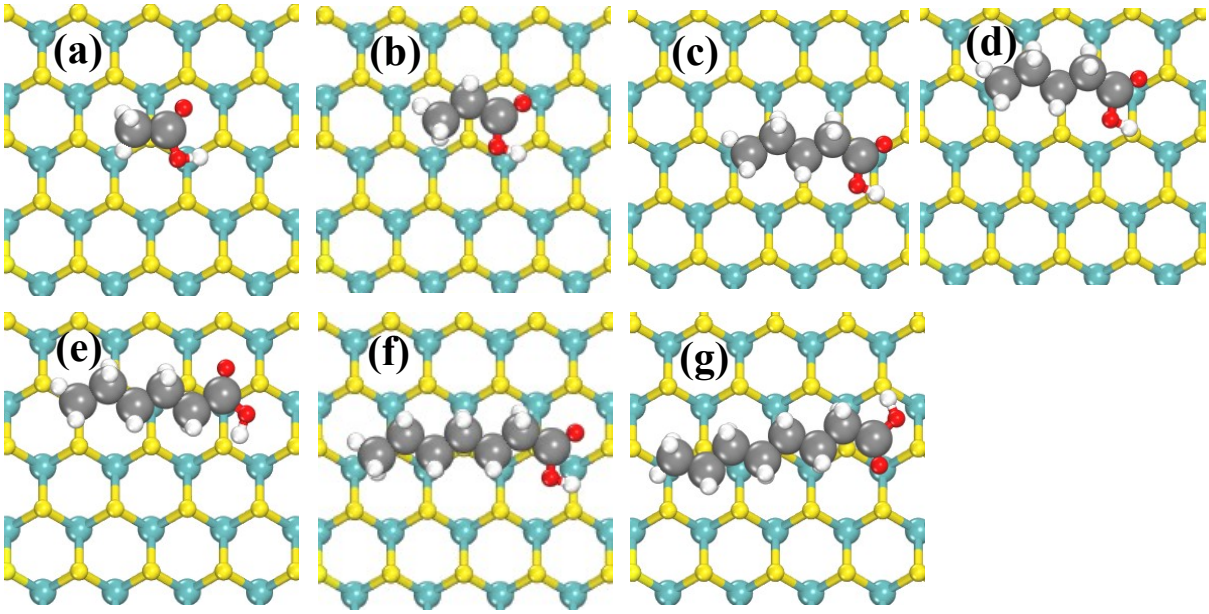

Fig. S3. Optimized structures of thermodynamically preferred models for carboxylic acid with different carbon chain on monolayer MoS_2.

Table S1. Calculated adsorption energy of eight types of VOC molecules (alkanes, aromatic hydrocarbon, alkynes, aldehydes, ketones, alkenes, alcohols and carboxylic acids) on the monolayer MoS_2.

Types	Adsorption Energy(eV)							
	Number of C atoms							
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Alkane	-	-0.34	-0.49	-0.62	-0.76	-0.88	-0.98	-1.14
aromatic hydrocarbon	-	-	-	-	-	-0.82	-0.99	-1.07
Alkyne	-	-0.32	-0.46	-0.59	-0.73	-0.86	-1.10	-1.07
Aldehydes	-0.25	-0.37	-0.49	-0.64	-0.71	-0.91	-1.03	-1.16
Ketone	-	-	-0.54	-0.65	-0.80	-0.91	-1.03	-1.18
Alkene	-	-0.37	-0.50	-0.58	-0.67	-0.91	-1.04	-1.18
Alcohols	-0.32	-0.44	-0.57	-0.65	-0.77	-0.96	-1.07	-1.12
carboxylic acid	-	-0.44	-0.57	-0.73	-0.78	-0.96	-1.08	-1.19

Table S2. The distance of VOCs with varying carbon chain lengths to the MoS_2 surface.

Types	$d^{\#}$ **(Å)**	d^{*} **(Å)**
$\mathbf{CH_3CH_3}$	3.42	3.41
$\mathbf{CH_3CH_2CH_3}$	3.39	3.39
$\mathbf{CH_3(CH_2)_2CH_3}$	3.40	3.24
$\mathbf{CH_3(CH_2)_3CH_3}$	3.39	3.43
$\mathbf{CH_3(CH_2)_4CH_3}$	3.44	3.41
$\mathbf{CH_3(CH_2)_5CH_3}$	3.47	3.48
$\mathbf{CH_3(CH_2)_6CH_3}$	3.45	3.49

$d^{\#}$: the average distance of VOCs to the MoS_2 surface.

d^{*} : the distance from the center of VOCs to the MoS_2 surface.