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Novel insights into the unique intrinsic sensing behaviors of 2D nanomaterials for volatile organic compounds: from graphene to MoS_2 and black phosphorous

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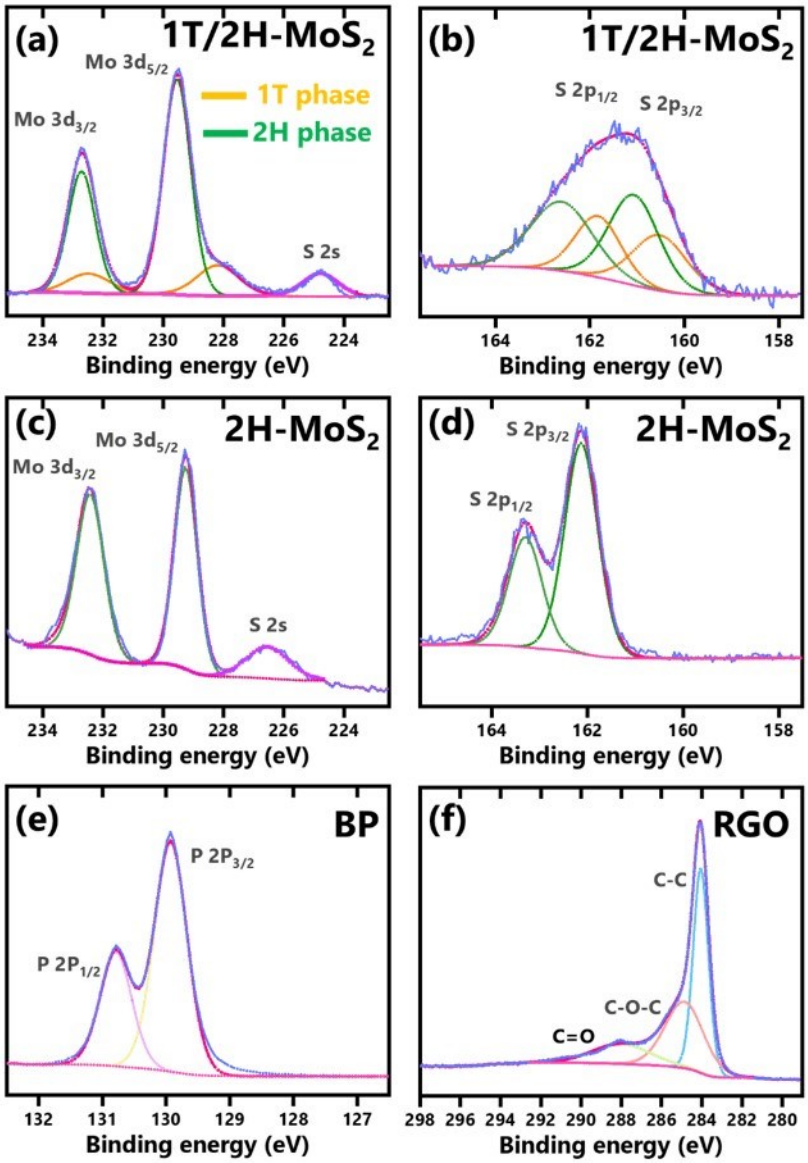


Figure S1 XPS spectra of (a)-(b) 1T/2H-MoS_2, (c)- (d) 2H-MoS_2, (e) BP, and (f) RGO. The orange and green line represents 1T and 2H phase of MoS_2, respectively.

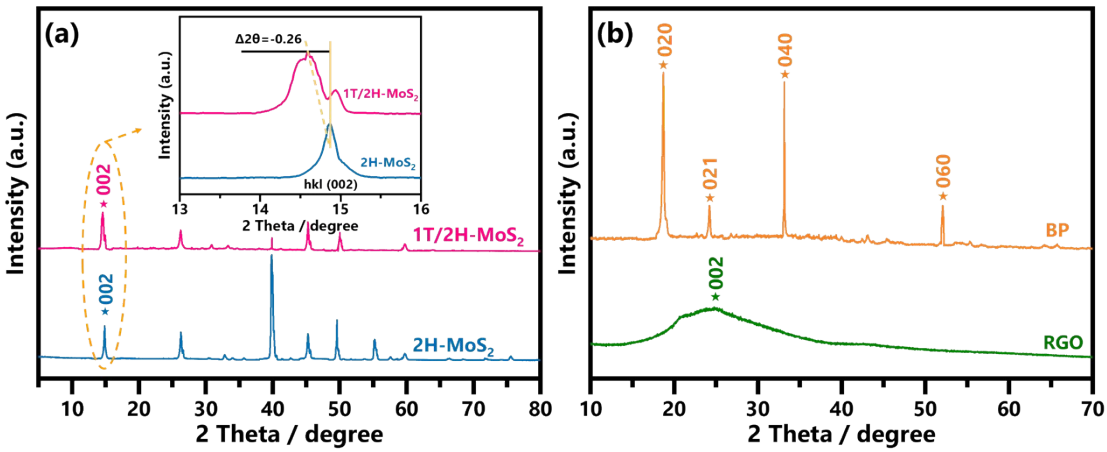


Figure S2 XRD patterns of (a) 1T/2H-MoS_2 and 2H-MoS_2, and (b) BP and RGO.

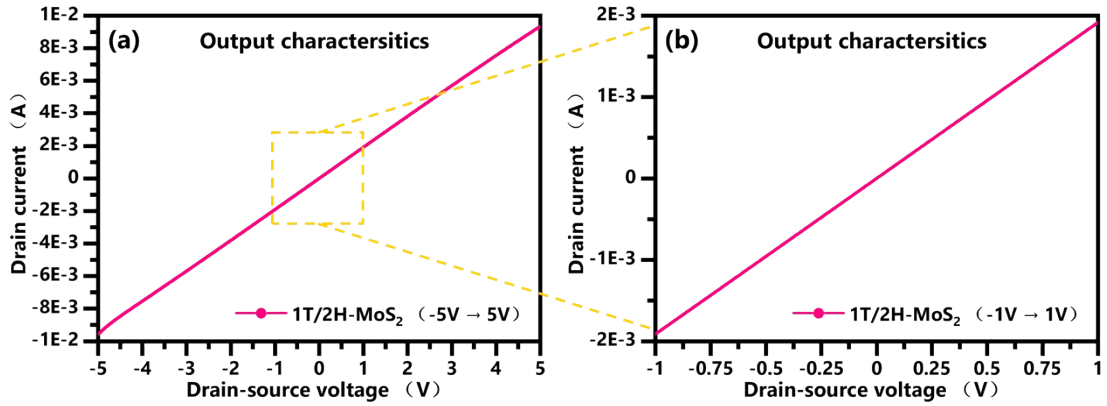


Figure S3 Drain current (I_{ds}) vs. source-drain voltage (V_{ds}) for 1T/2H-MoS_2 with a voltage range of (a) -5 V to +5 V and (b) -1 V to +1 V, respectively.

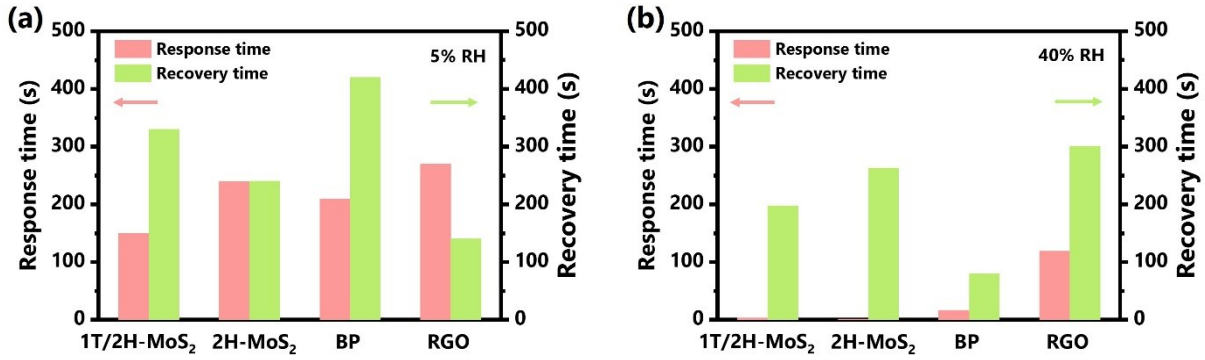


Figure S4 Comparison of response and recovery times of 1T/2H-MoS_2, 2H-MoS_2, BP, and RGO sensor toward 1 ppm HCHO in dry air and under 40% RH.

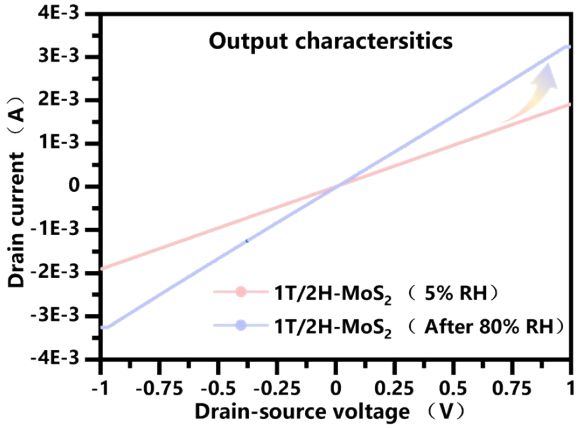


Figure S5 The I_{ds}-V_{ds} of 1T/2H-MoS_2 before and after sensing tests under humidity condition.

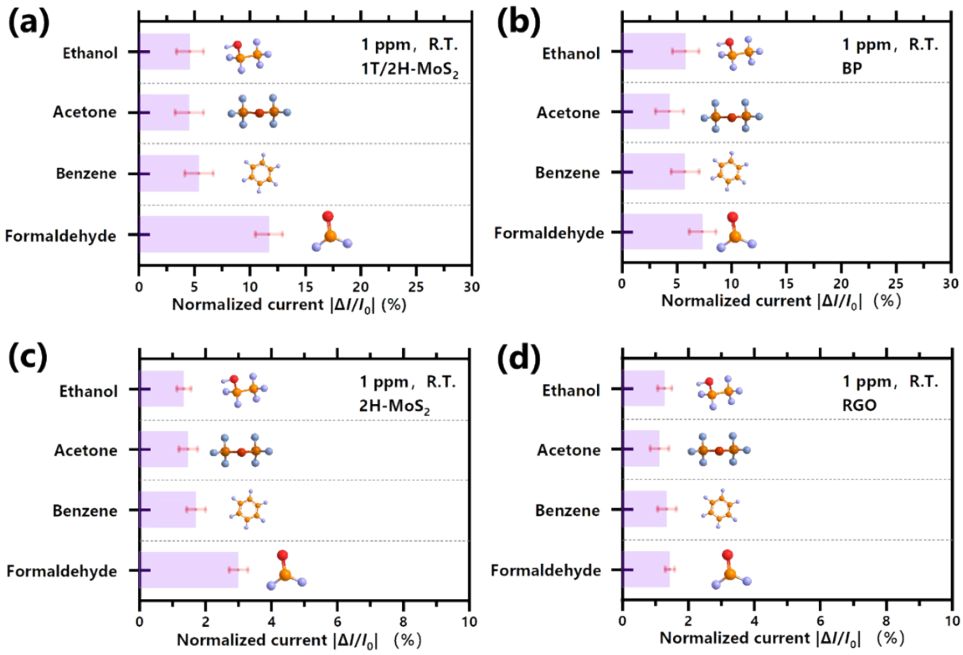


Figure S6 Relative responses of the (a) 1T/2H-MoS_2, (b) BP, (c) 2H-MoS_2 and (d) RGO FET sensors to different VOCs at 1 ppm.

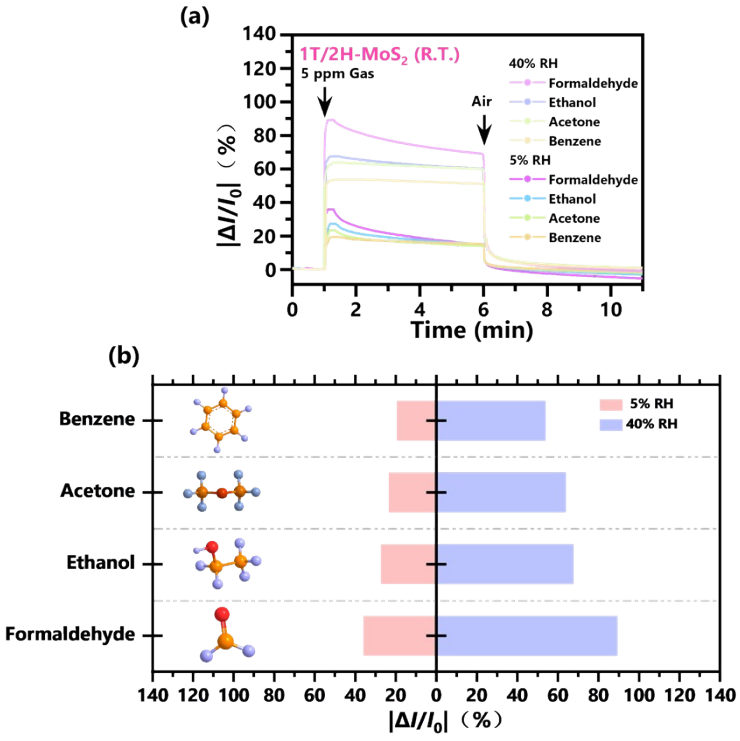
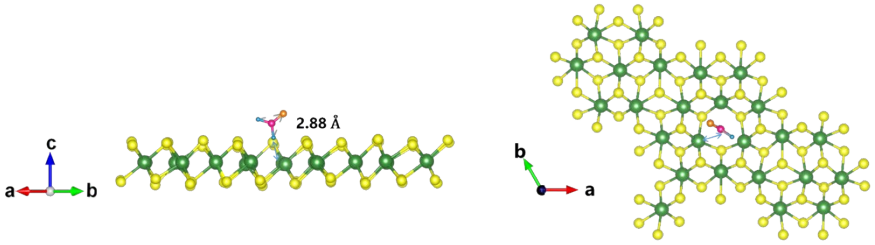
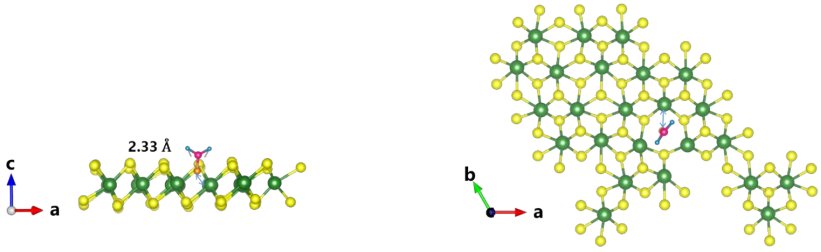


Figure S7 (a) Gas sensing responses and (b) relative responses of 1T/2H-MoS_2 sensor to different VOCs at 5 ppm under 5% and 40% RH.

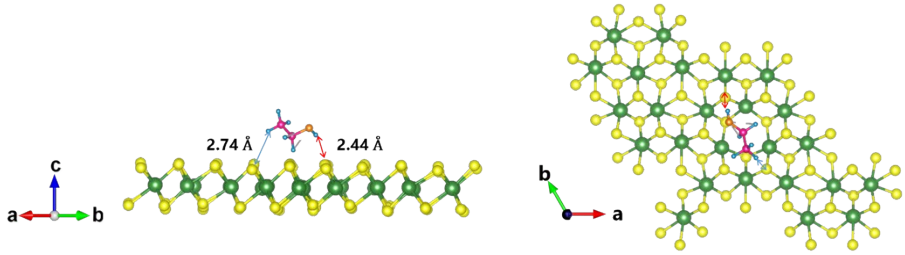
(a) 1T-MoS_2→ Formaldehyde - H terminate



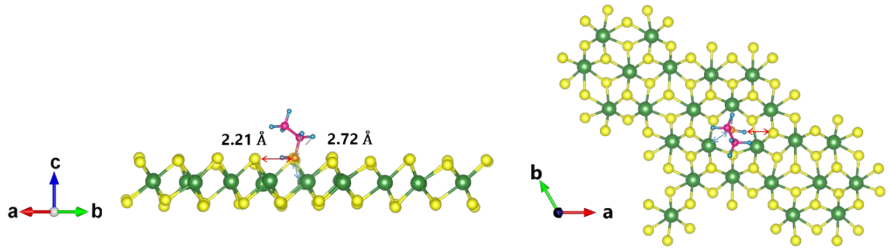
(b) 1T-MoS_2→ Formaldehyde - O terminate



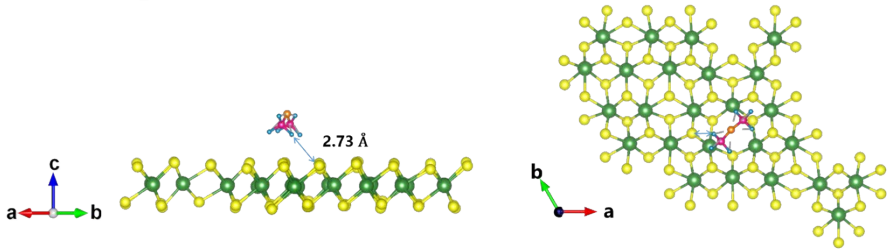
(c) 1T-MoS_2→ Ethanol - H terminate



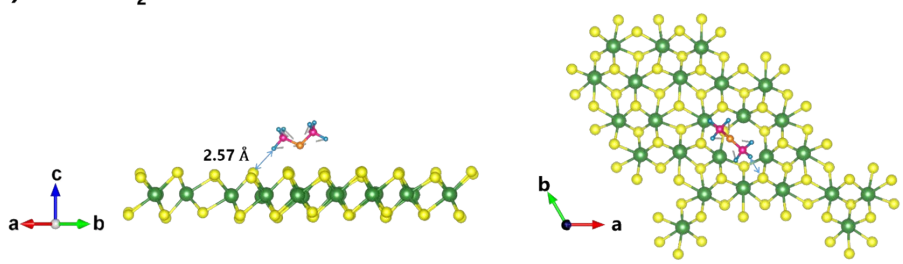
(d) 1T-MoS_2→ Ethanol - O terminate



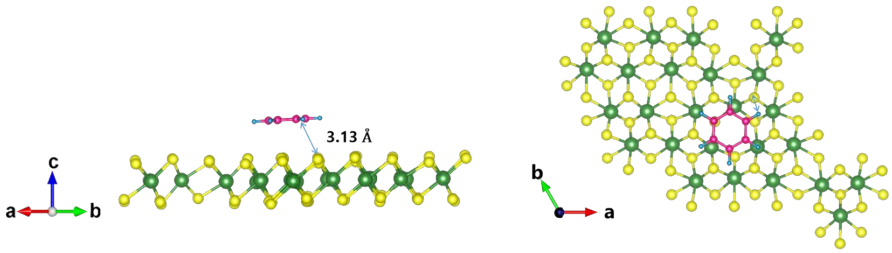
(e) 1T-MoS_2→ Acetone - H terminate



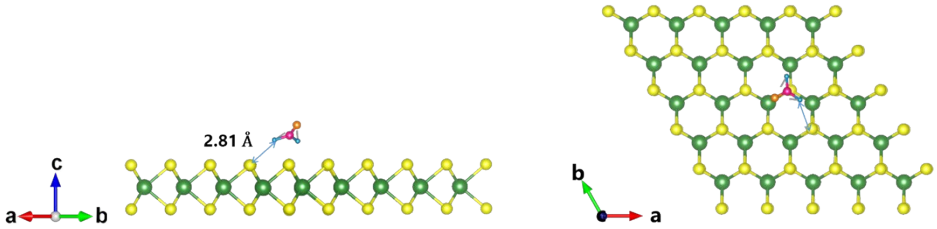
(f) 1T-MoS_2→ Acetone - O terminate



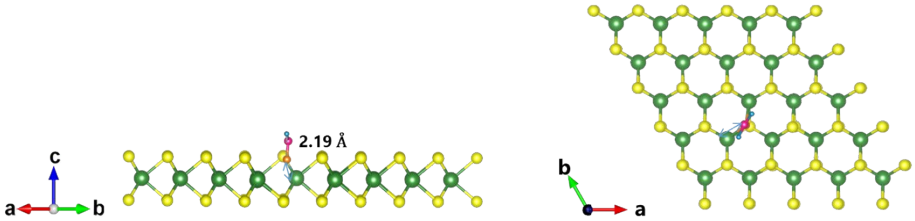
(g) 1T-MoS_2→ Benzene - H terminate



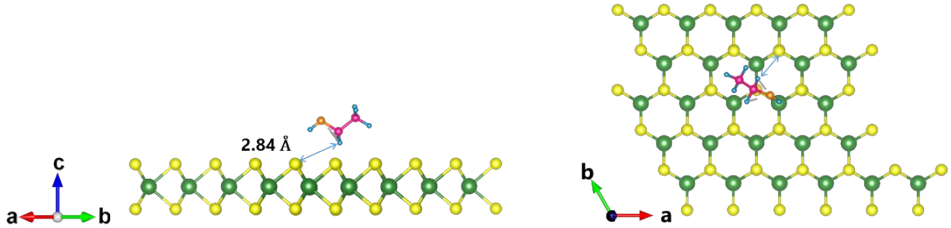
(h) 2H-MoS_2→ Formaldehyde - H terminate



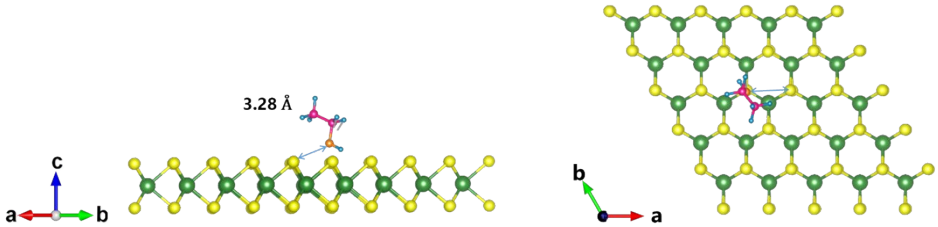
(i) 2H-MoS_2→ Formaldehyde - O terminate



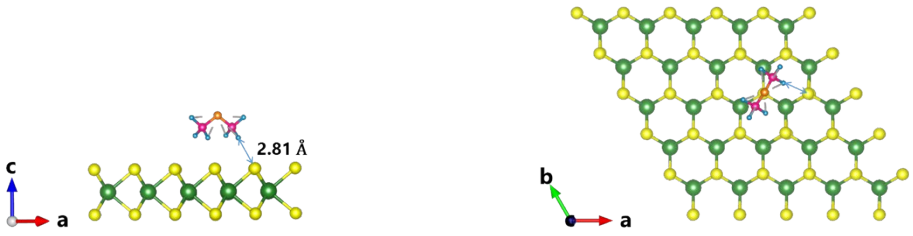
(j) 2H-MoS_2→ Ethanol - H terminate



(k) 2H-MoS_2→ Ethanol - O terminate



(l) 2H-MoS_2→ Acetone - H terminate



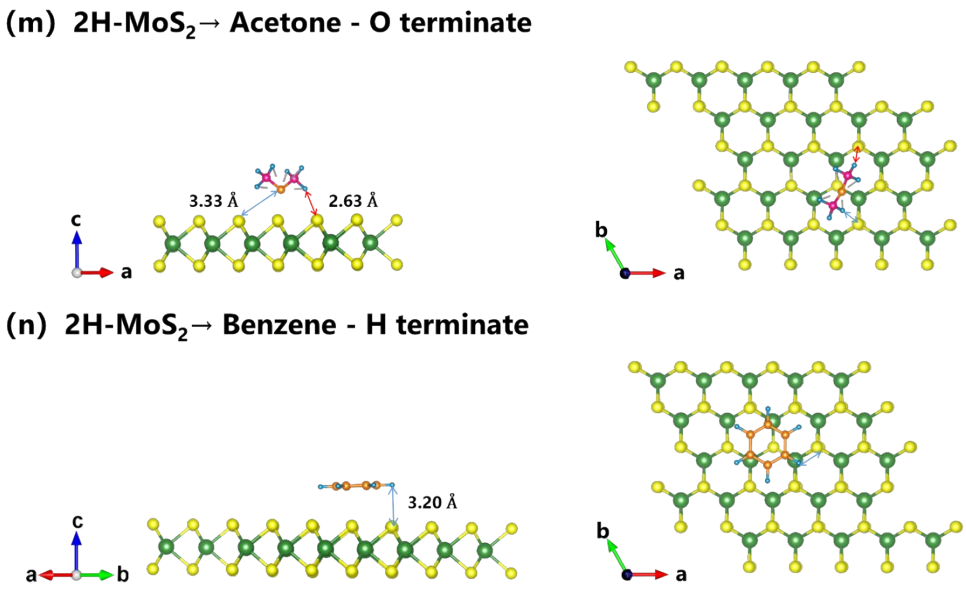
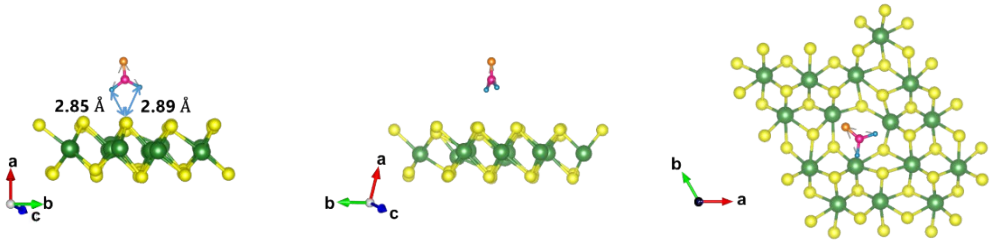


Figure S8 Configurations of (a, b) formaldehyde, (c, d) ethanol, (e, f) acetone, (g, h) benzene gas molecule adsorbed with H terminate and O terminate, respectively, at the sulfur vacancy of 1T-MoS_2. Configurations of (h, i) formaldehyde, (j, k) ethanol, (l, m) acetone, (n) benzene gas molecule adsorbed with H terminate and O terminate, respectively, at the sulfur vacancy of 2H-MoS_2.

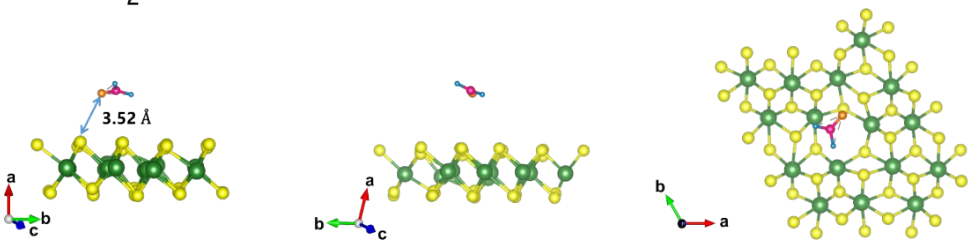
Table S1 DFT calculation results of adsorption energy (eV) of formaldehyde, ethanol, acetone, benzene molecule with H atom or O atom as terminate on sulfur vacancy site on 1T-MoS_2 and 2H-MoS_2. The "H" and "O" refer to the bonding approaches for analyte molecule adsorbed at the S vacancy that rely on H or O atom, respectively.

Channel	Formaldehyde-H	Formaldehyde-O	Ethanol-H	Ethanol-O	Acetone-H	Acetone-O	Benzene-H
1T-MoS_2	-0.744	-1.645	-0.846	-1.213	-0.715	-0.778	-0.954
2H-MoS_2	-0.287	-0.557	-0.381	-0.386	-0.325	-0.329	-0.568

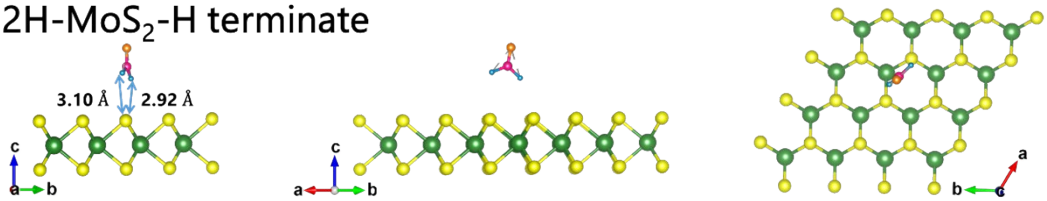
(a) 1T-MoS_2-H terminate



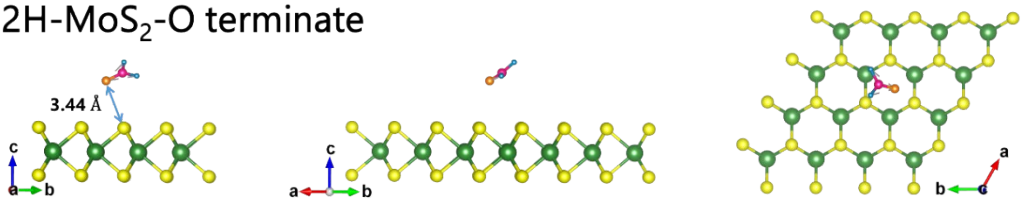
(b) 1T-MoS_2-O terminate



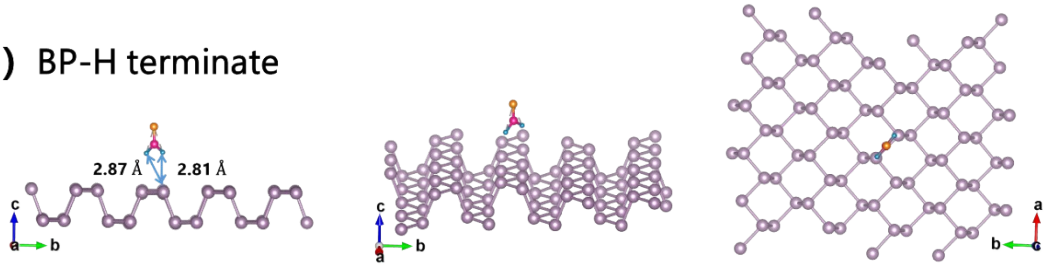
(c) 2H-MoS_2-H terminate



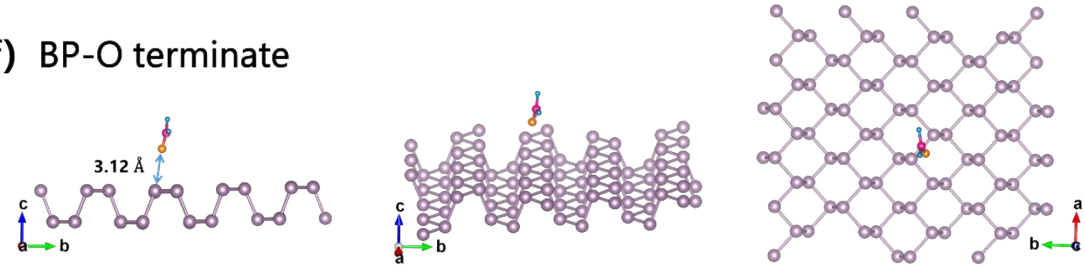
(d) 2H-MoS_2-O terminate



(e) BP-H terminate



(f) BP-O terminate



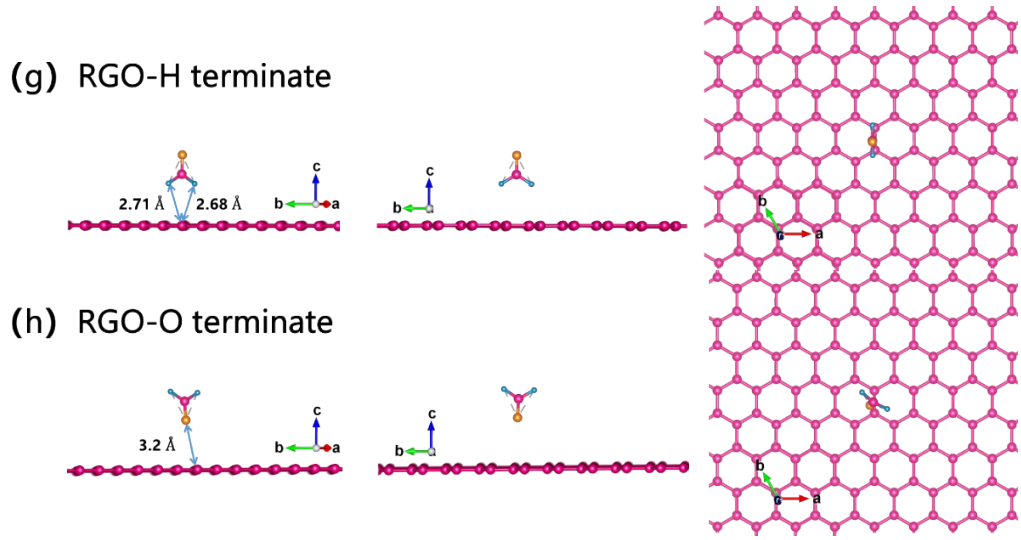


Figure S9 Configurations of HCHO molecule adsorbed with H atoms as terminate at the basal plane of (a) 1T-MoS_2, (c) 2H-MoS_2, (e) BP, (g) RGO, and with O atom as terminate at the basal plane of (b) 1T-MoS_2, (d) 2H-MoS_2, (f) BP, (h) RGO.

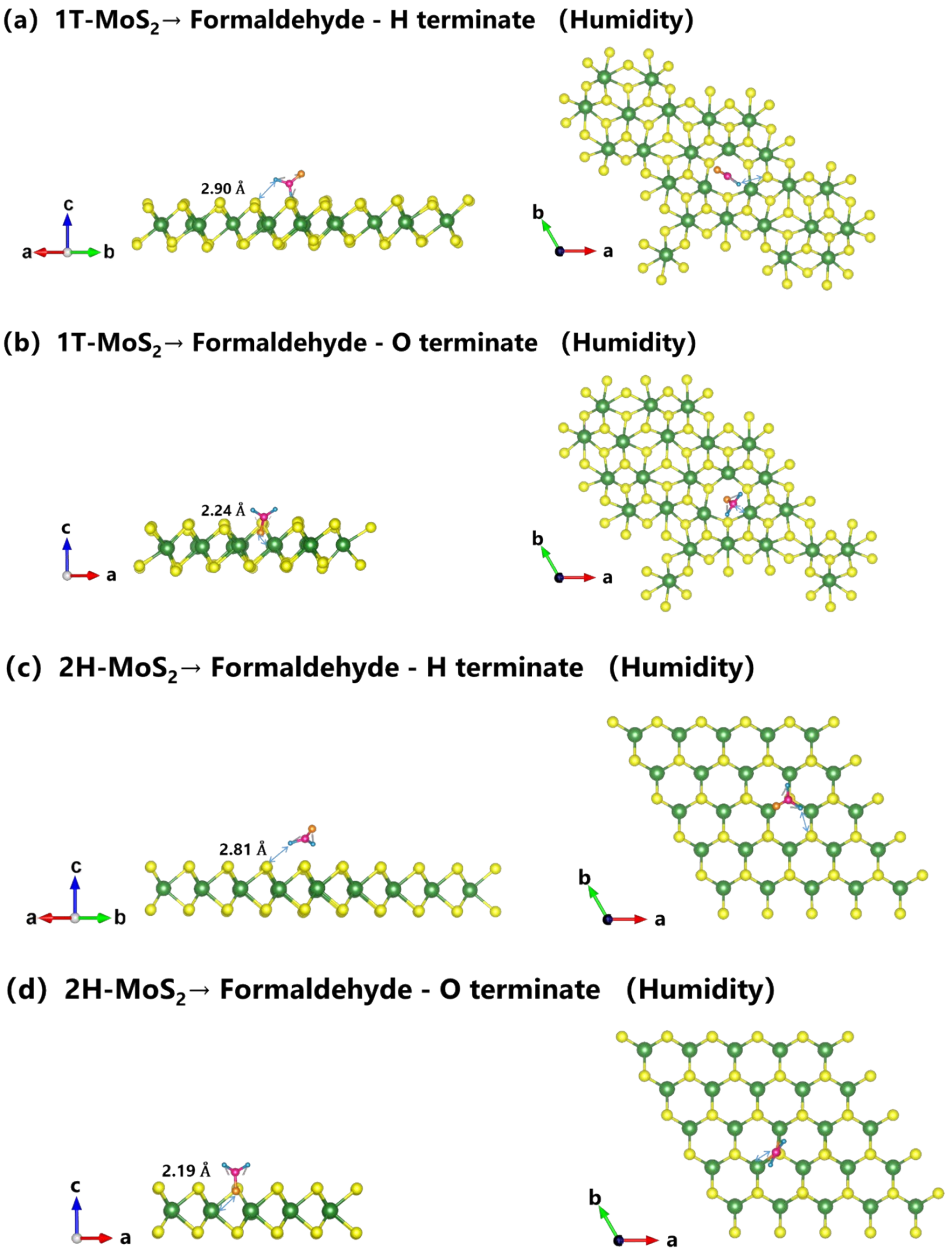


Figure S10 Configurations of formaldehyde molecule adsorbed with H atoms as terminate at the sulfur vacancy of (a) 1T-MoS_2, (c) 2H-MoS_2; and with O atoms as terminate at the sulfur vacancy of (b) 1T-MoS_2, (d) 2H-MoS_2 under humidity condition.

Table S2 DFT calculation results of adsorption energy (eV) of formaldehyde molecule with H atom or O atom as terminate, respectively, on sulfur vacancy sites on 1T-MoS_2 and 2H-MoS_2 under humidity condition. The "H" and "O" refer to the bonding approaches for analyte molecule adsorbed at the S vacancy that rely on H or O atom, respectively.

Channel	Formaldehyde-H (humidity)	Formaldehyde–O (humidity)
1T-MoS_2	-0.864	-1.917
2H-MoS_2	-0.426	-0.609