

## Electronic Supplementary Information

### Investigation of the interfacial behavior of organics on the sulfide semiconductor surface by quantum chemical calculation and molecular dynamic simulation

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Table. S1 the surface of the sulfide semiconductor used in the experiment

semiconductor	CdS	CdS	ZnS	MoS <sub>2</sub>	SnS
surface	(1,1,1)	(1,0,1)	(1,1,1)	(0,0,2)	(1,1,1)

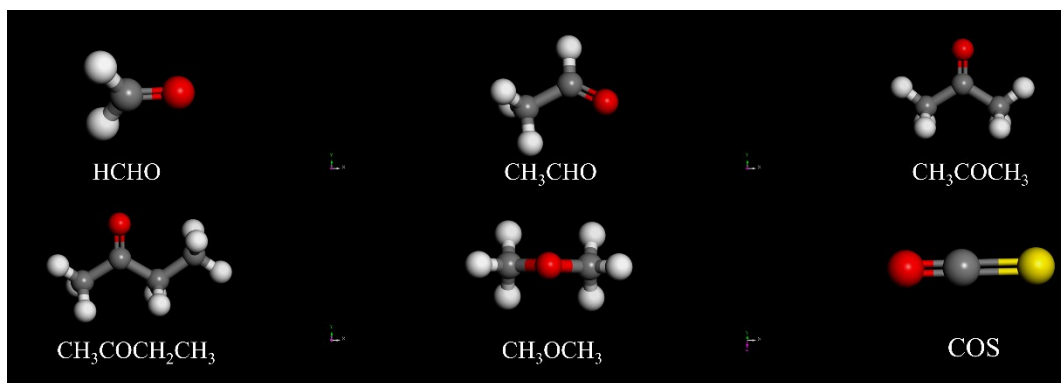


Fig. S1 ball and stick models of HCHO, CH<sub>3</sub>CHO, CH<sub>3</sub>COCH<sub>3</sub>, CH<sub>3</sub>COCH<sub>2</sub>CH<sub>3</sub>, CH<sub>3</sub>OCH<sub>3</sub>, COS

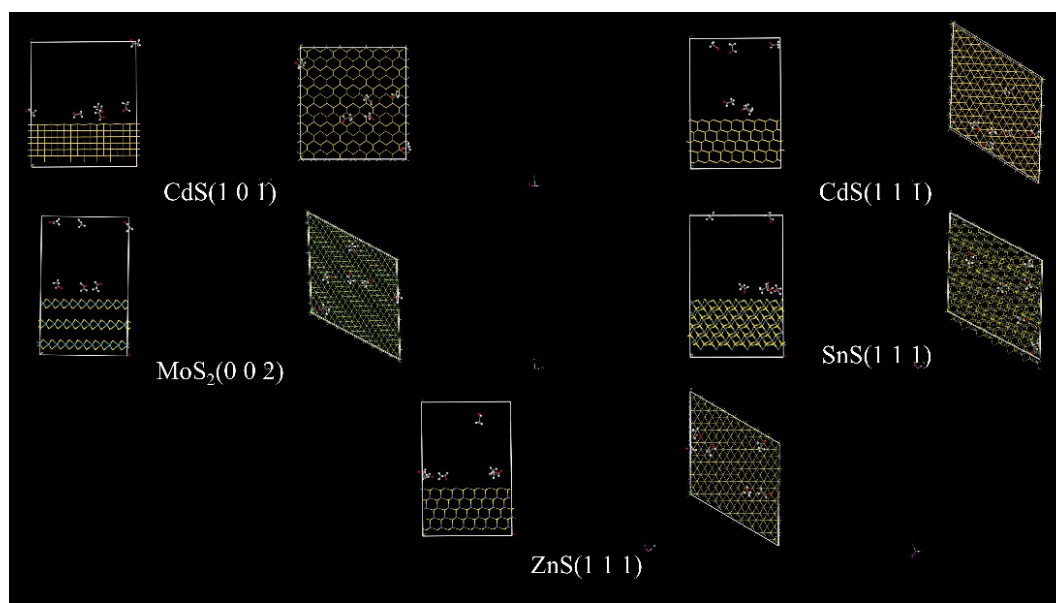


Fig. S2 The final configuration of the simulation box with gas phase CH<sub>3</sub>CHO molecule on sulfide semiconductors.

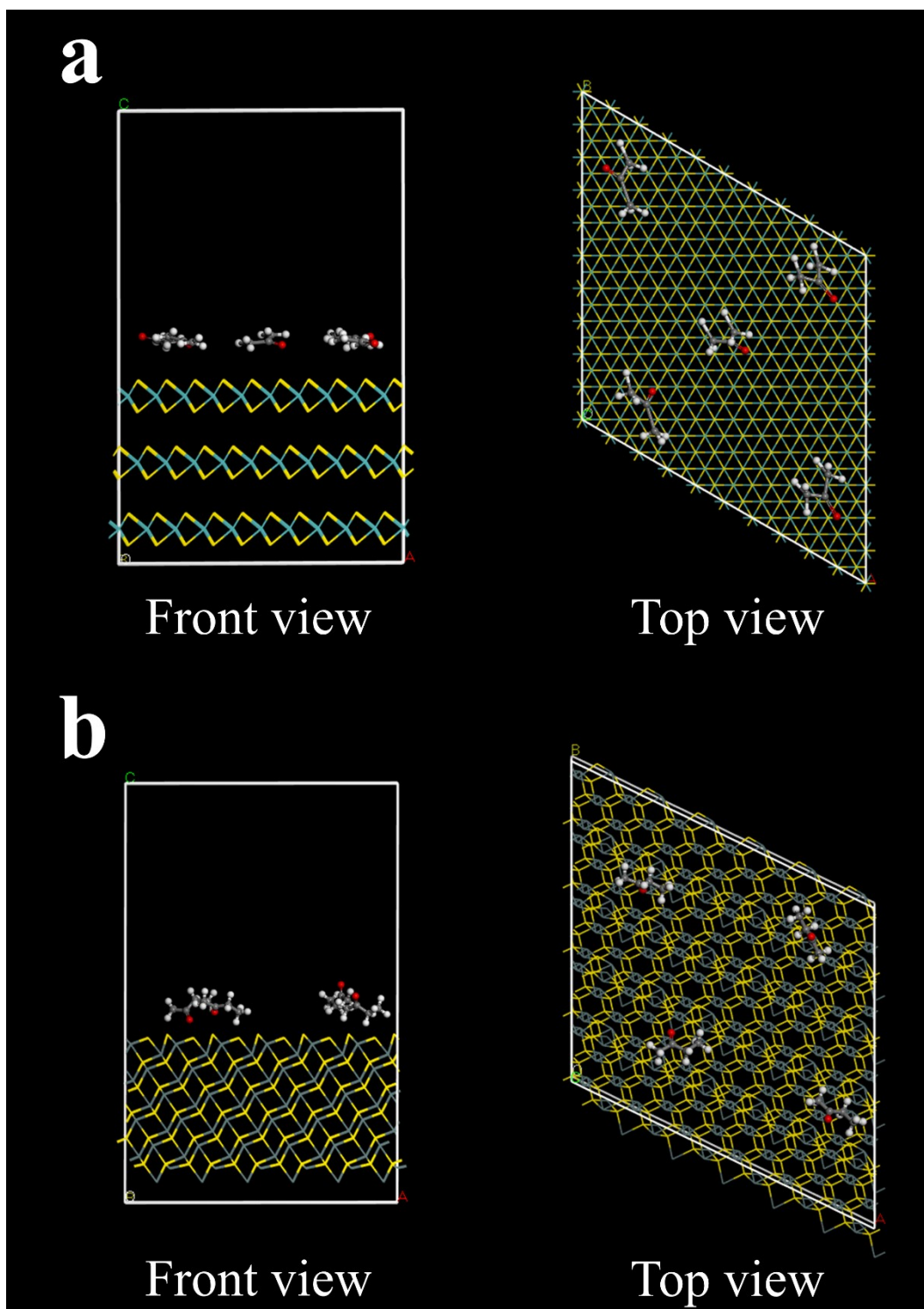


Fig. S3 a. The initial state of the simulation box containing  $\text{CH}_3\text{COCH}_3$  molecules and  $\text{MoS}_2$  (0 0 2) semiconductors; b. The initial state of the simulation box containing  $\text{CH}_3\text{COCH}_2\text{CH}_3$  molecules and  $\text{SnS}$  (1 1 1) semiconductors

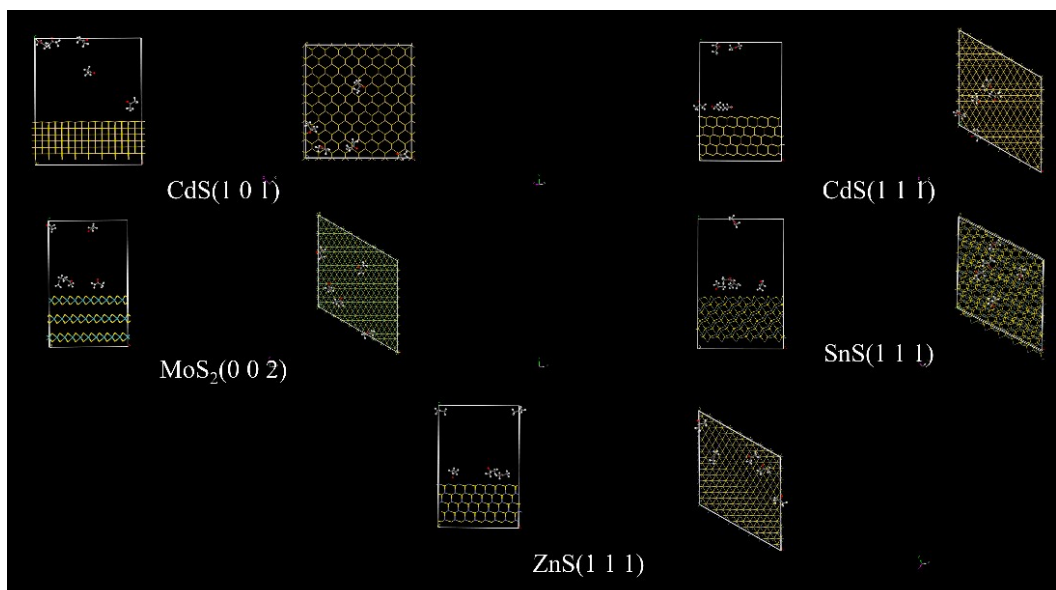


Fig. S4 The final configuration of the simulation box with gas phase  $\text{CH}_3\text{COCH}_3$  molecule on sulfide semiconductors.

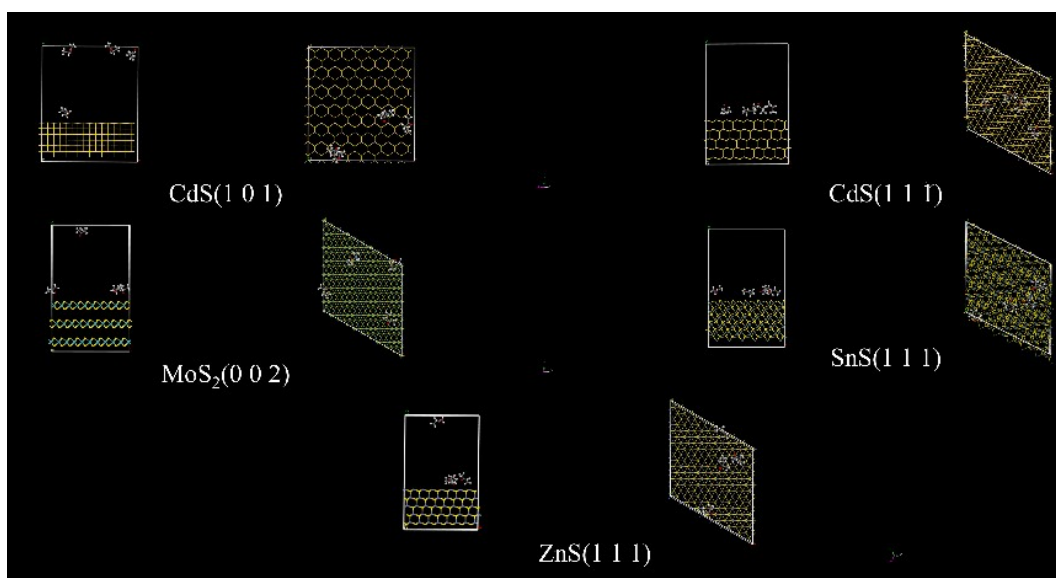


Fig. S5 The final configuration of the simulation box with gas phase  $\text{CH}_3\text{COCH}_2\text{CH}_3$  molecule on sulfide semiconductors.

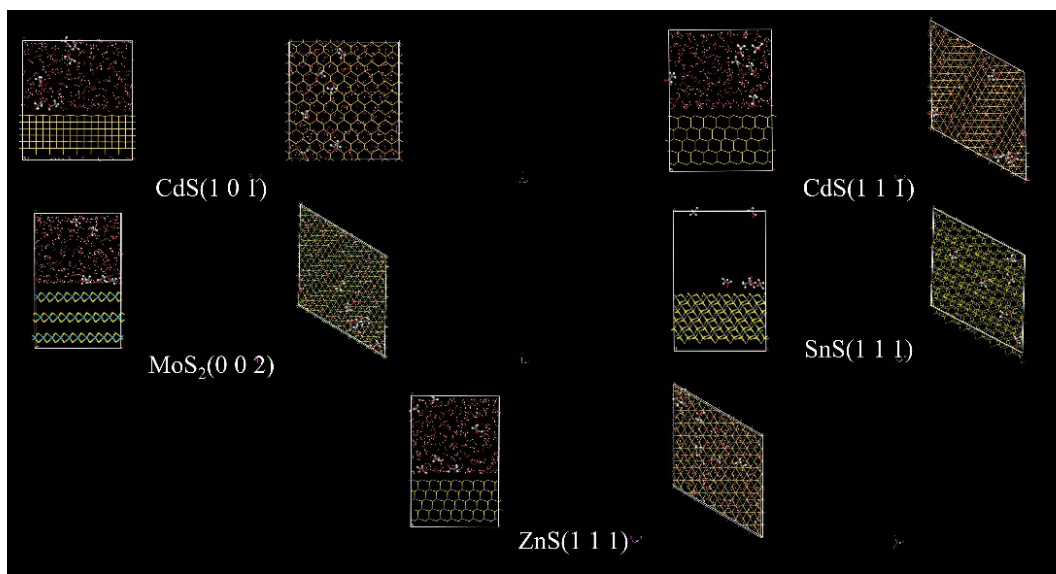


Fig. S6 The final configuration of the simulation box with water phase  $\text{CH}_3\text{CHO}$  molecule on sulfide semiconductors.

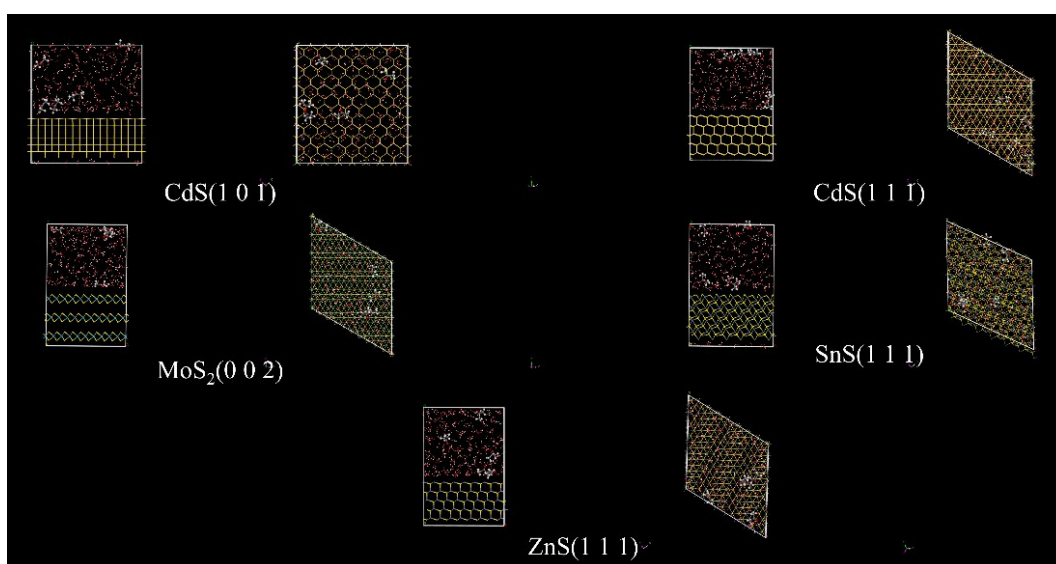


Fig. S7 The final configuration of the simulation box with water phase  $\text{CH}_3\text{COCH}_3$  molecule on sulfide semiconductors.

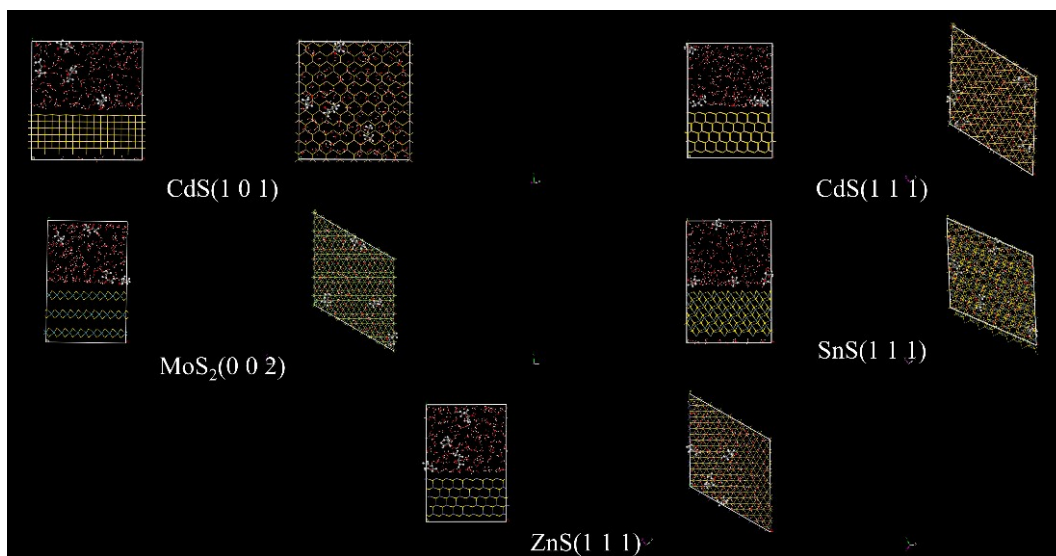


Fig. S8 The final configuration of the simulation box with water phase  $\text{CH}_3\text{COCH}_2\text{CH}_3$  molecule on sulfide semiconductors.

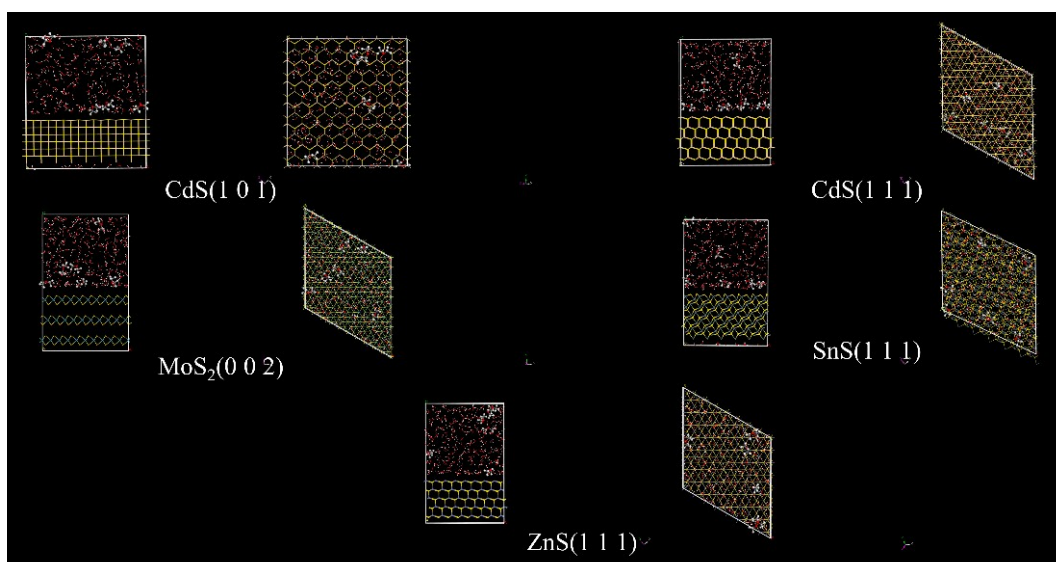


Fig. S9 The final configuration of the simulation box with water phase  $\text{CH}_3\text{OCH}_3$  molecule on sulfide semiconductors.



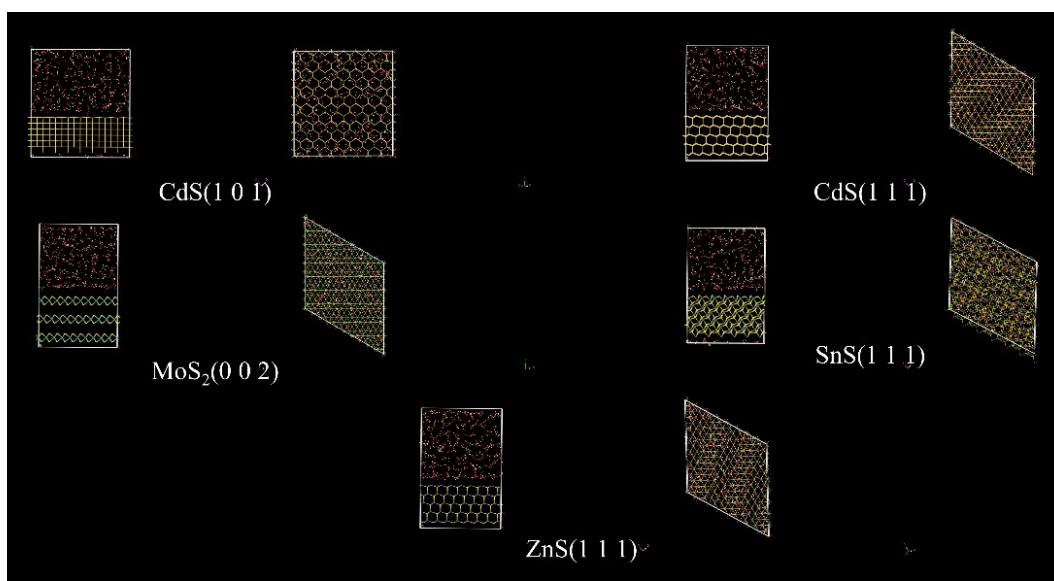


Fig. S10 The final configuration of the simulation box with water phase COS molecule on sulfide semiconductors.

Table S2 Experimental results of adsorption of HCHO molecules on the surface of various sulfide semiconductor materials in gas phase conditions

semiconductors	Cut crystal face	Total energy (kcal/mol)	semiconductors energy (kcal/mol)	HCHO energy (kcal/mol)	Adsorption energy (kcal/mol)
CdS	111	4530.6	4523.1	14.276	-6.776
CdS	101	4124.2	4111.6	16.709	-4.109
MoS <sub>2</sub>	002	49888	49880	18.576	-10.576
SnS	111	45780	45768	24.518	-12.518
ZnS	111	3925.2	3919.6	10.290	-4.690

Table S3 Experimental results of adsorption of CH<sub>3</sub>CHO molecules on the surface of various sulfide semiconductor materials in the gas phase

semiconductors	Cut crystal face	Total energy (kcal/mol)	semiconductors energy (kcal/mol)	HCHO energy (kcal/mol)	Adsorption energy (kcal/mol)
CdS	111	4551.0	4523.4	30.750	-3.150
CdS	101	4132.5	4111.6	33.104	-12.204
MoS <sub>2</sub>	002	49889	49880	27.673	-18.673
SnS	111	45780	45766	36.074	-22.074
ZnS	111	3936.2	3919.5	27.449	-10.749

Table S4 Experimental results of adsorption of CH<sub>3</sub>COCH<sub>3</sub> molecules on the surface of various sulfide semiconductor materials in the gas phase

semiconductors	Cut crystal face	Total energy (kcal/mol)	semiconductors energy (kcal/mol)	CH <sub>3</sub> COCH <sub>3</sub> energy (kcal/mol)	Adsorption energy (kcal/mol)
CdS	111	4555.0	4522.8	46.370	-14.170
CdS	101	4138.6	4111.4	39.520	-12.320
MoS <sub>2</sub>	002	49898	49880	42.574	-24.574
SnS	111	45785	45766	43.052	-24.052
ZnS	111	3944.4	3919.2	39.483	-14.283

Table S5 Experimental results of adsorption of CH<sub>3</sub>COCH<sub>2</sub>CH<sub>3</sub> molecules on the surface of various sulfide semiconductor materials in the gas phase

semiconductors	Cut crystal face	Total energy (kcal/mol)	semiconductors energy (kcal/mol)	CH <sub>3</sub> COCH <sub>2</sub> CH <sub>3</sub> energy (kcal/mol)	Adsorption energy (kcal/mol)
CdS	111	4551.6	4522.8	50.042	-21.242
CdS	101	4158.7	4111.4	55.611	-8.311
MoS <sub>2</sub>	002	49908	49880	45.878	-17.878
SnS	111	45777	45766	45.063	-34.063
ZnS	111	3970.9	3919.2	60.952	-9.252

Table S6 Experimental results of adsorption of CH<sub>3</sub>OCH<sub>3</sub> molecules on the surface of various sulfide semiconductor materials in the gas phase

semiconductors	Cut crystal face	Total energy (kcal/mol)	semiconductors energy (kcal/mol)	CH <sub>3</sub> OCH <sub>3</sub> energy (kcal/mol)	Adsorption energy (kcal/mol)
CdS	111	4575.5	4523.2	66.664	-14.364
CdS	101	4166.3	4111.7	69.648	-15.048
MoS <sub>2</sub>	002	49926	49880	61.511	-15.511
SnS	111	45807	45768	63.945	-24.945
ZnS	111	3977.7	3919.7	65.774	-7.774



Table S7 Experimental results of adsorption of COS molecules on the surface of various sulfide semiconductor materials in the gas phase

semiconductors	Cut crystal face	Total energy (kcal/mol)	semiconductors energy (kcal/m ol)	COS energy (kcal/m ol)	Adsorption energy (kcal/mol)
CdS	111	4522.5	4523.1	5.7532	-6.353
CdS	101	4111.6	4111.6	6.7370	-6.737
MoS <sub>2</sub>	002	49873	49880	4.6656	-11.666
SnS	111	45756	45767	10.838	-21.838
ZnS	111	3918.5	3919.5	8.6393	-9.639

Table S8 Experimental results of adsorption of HCHO molecules on the surface of various sulfide semiconductor materials in the water phase

semiconductors	Cut crystal face	Total energy (kcal/mol)	semiconductors energy (kcal/m ol)	HCHO energy (kcal/m ol)	Adsorption energy (kcal/mol)
CdS	111	4524.4	4523.5	10.119	-9.219
CdS	101	4114.2	4112.3	10.747	-8.847
MoS <sub>2</sub>	002	49879	49881	12.055	-14.055
SnS	111	45766	45769	12.664	-15.664
ZnS	111	3925.4	3919.6	13.141	-7.341

Table S9 Experimental results of adsorption of CH<sub>3</sub>CHO molecules on the surface of various sulfide semiconductor materials in the water phase

semiconductors	Cut crystal face	Total energy (kcal/mol)	semiconductors energy (kcal/m ol)	CH <sub>3</sub> CHO energy (kcal/m ol)	Adsorption energy (kcal/mol)
CdS	111	4535.5	4523.5	25.309	-13.309
CdS	101	4126.6	4112.4	26.845	-12.645
MoS <sub>2</sub>	002	49890	49881	28.410	-19.410
SnS	111	45773	45769	34.585	-30.585
ZnS	111	3931.3	3919.6	23.270	-11.570

Table S10 Experimental results of adsorption of CH<sub>3</sub>COCH<sub>3</sub> molecules on the surface of various sulfide semiconductor materials in the water phase

semiconductors	Cut crystal face	Total energy (kcal/mol)	semiconductors energy (kcal/m ol)	CH <sub>3</sub> COCH <sub>3</sub> energy (kcal/m ol)	Adsorption energy (kcal/mol)
CdS	111	4539.4	4523.6	37.310	-21.510
CdS	101	4140.0	4112.4	38.343	-10.743
MoS <sub>2</sub>	002	49897	49881	37.223	-21.223
SnS	111	45781	45769	40.026	-28.026
ZnS	111	3938.4	3919.6	39.650	-20.850

Table S11 Experimental results of adsorption of CH<sub>3</sub>COCH<sub>2</sub>CH<sub>3</sub> molecules on the surface of various sulfide semiconductor materials in the water phase

semiconductors	Cut crystal face	Total energy (kcal/mol)	semiconductors energy (kcal/m ol)	CH <sub>3</sub> COCH <sub>2</sub> CH <sub>3</sub> energy (kcal/m ol)	Adsorption energy (kcal/mol)
CdS	111	4563.7	4523.7	58.098	-18.098
CdS	101	4131.9	4096.7	51.249	-16.049
MoS <sub>2</sub>	002	49904	49881	47.053	-24.053
SnS	111	45784	45770	46.832	-32.832
ZnS	111	3947.6	3919.8	48.039	-20.239

Table S12 Experimental results of adsorption of CH<sub>3</sub>OCH<sub>3</sub> molecules on the surface of various sulfide semiconductor materials in the water phase

semiconductors	Cut crystal face	Total energy (kcal/mol)	semiconductors energy (kcal/m ol)	CH <sub>3</sub> OCH <sub>3</sub> energy (kcal/m ol)	Adsorption energy (kcal/mol)
CdS	111	4578.1	4523.7	71.380	-16.980
CdS	101	4162.2	4112.5	64.816	-15.116
MoS <sub>2</sub>	002	49922	49881	66.591	-25.591
SnS	111	45807	45770	73.837	-36.837
ZnS	111	3967.2	3919.8	64.925	-17.525

Table S13 Experimental results of adsorption of COS molecules on the surface of various sulfide semiconductor materials in the water phase

semiconductors	Cut crystal face	Total energy (kcal/mol)	semiconductors energy (kcal/m ol)	COS energy (kcal/m ol)	Adsorption energy (kcal/mol)
CdS	111	4517.0	4523.7	0.035869	-6.736
CdS	101	4109.3	4112.5	0.026119	-3.226
MoS <sub>2</sub>	002	49867	49881	0.10562	-14.106
SnS	111	45756	45770	0.065389	-14.065
ZnS	111	3909.2	3919.8	-0.19577	-10.4043