

## Supplementary Information

### **A first-principles study on Ni-decorated MoS<sub>2</sub> for efficient formaldehyde degradation over a wide temperature range**

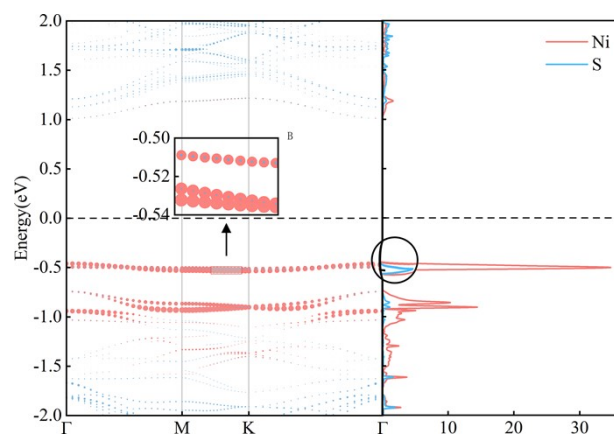
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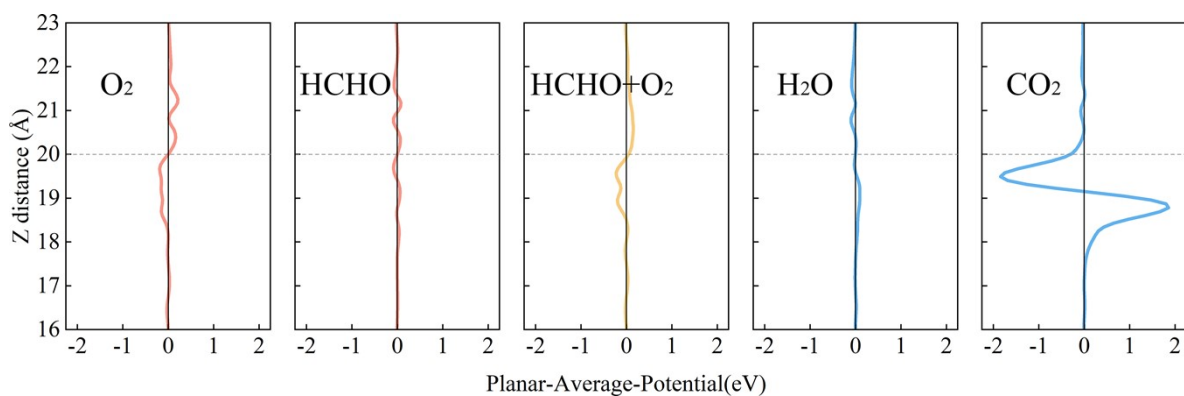
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**Fig. S1** Projected band structure and projected DOS of Ni-MoS<sub>2</sub>.



**Fig. S2** Planar-Average-Potential plot illustrating the adsorption behavior of gas molecules on the Ni-MoS<sub>2</sub> surface. The red line represents the reactant species (HCHO and O<sub>2</sub> molecules), while the blue line corresponds to the product species (H<sub>2</sub>O and CO<sub>2</sub> molecules). Additionally, the yellow line depicts the coadsorption of HCHO and O<sub>2</sub> molecules. The dashed gray line indicates the position of the Ni atom.

**Table S1** The logarithms of reaction rate constants for the rate-determining steps in each pathway within the temperature range of 100K to 800K.

Temperature (K)	L-H (PATH1)	L-H (PATH2)	E-R (PATH1)	E-R (PATH2)
100	27.99664332	28.98648952	28.89216	29.17047
200	30.63161661	31.08865637	31.08101	31.2131
300	31.86106112	32.13268705	32.15475	32.17468
400	32.64710373	32.82307908	32.86152	32.84793
500	33.22073434	33.33781595	33.40108	33.35264
600	33.67092521	33.74777171	33.82061	33.75604
700	34.04080822	34.08819785	34.16827	34.09185
800	34.35441865	34.39110677	34.46496	34.37938

**Table S2** The imaginary frequency values of transition states ( $\text{cm}^{-1}$ ).

	TS1	TS2	TS3	TS4	TS5	TS6	TS7	TS8	TS9
Frequency	80.51	374.15	88.32	361.80	111.70	114.85	205.76	151.78	42.93

**Table S3** The coordinates of optimized transition state configurations [(a)~(i): TS1~TS9].

(a)							(b)							(c)						
10.96	0.00	0.00					10.97	0.00	0.00					10.97	0.00	0.00				
-5.48	9.51	0.00					-5.48	9.51	0.00					-5.49	9.51	0.00				
-0.01	-0.01	26.55					0.00	-0.02	26.56					-0.05	0.04	26.55				
S	Mo	Ni	O	C	H		S	Mo	Ni	O	C	H		S	Mo	Ni	O	C	H	
24	12	1	3	1	2		24	12	1	3	1	2		24	12	1	3	1	2	
<b>Direct</b>							<b>Direct</b>							<b>Direct</b>						
0.17	0.50	0.56					0.17	0.50	0.56					0.18	0.50	0.56				
0.51	0.17	0.56					0.51	0.17	0.56					0.51	0.17	0.56				
0.84	0.84	0.56					0.84	0.84	0.56					0.84	0.83	0.56				
0.17	0.00	0.56					0.17	0.00	0.56					0.17	1.00	0.56				
0.51	0.67	0.56					0.51	0.67	0.56					0.51	0.67	0.56				
0.84	0.33	0.56					0.84	0.34	0.56					0.84	0.33	0.56				
0.01	0.17	0.56					0.01	0.17	0.56					0.01	0.17	0.56				
0.34	0.83	0.56					0.34	0.83	0.56					0.34	0.83	0.56				
0.67	0.50	0.56					0.67	0.50	0.56					0.67	0.50	0.56				
0.17	0.50	0.68					0.17	0.50	0.68					0.17	0.50	0.68				
0.51	0.17	0.68					0.51	0.17	0.68					0.51	0.17	0.68				
0.84	0.84	0.68					0.84	0.83	0.68					0.85	0.83	0.68				
0.17	0.00	0.68					0.17	0.00	0.68					0.17	0.00	0.68				
0.51	0.68	0.68					0.50	0.66	0.68					0.50	0.66	0.68				
0.84	0.33	0.68					0.84	0.34	0.68					0.84	0.33	0.68				
0.01	0.17	0.68					0.01	0.17	0.68					0.01	0.17	0.68				
0.34	0.84	0.68					0.34	0.84	0.68					0.34	0.83	0.68				
0.68	0.50	0.68					0.67	0.50	0.68					0.67	0.50	0.68				
0.01	0.67	0.56					0.01	0.67	0.56					0.01	0.67	0.56				
0.34	0.34	0.56					0.34	0.34	0.56					0.34	0.33	0.56				
0.67	0.00	0.56					0.67	1.00	0.56					0.67	1.00	0.56				
0.01	0.67	0.68					0.01	0.67	0.68					0.01	0.67	0.68				
0.33	0.33	0.68					0.34	0.33	0.68					0.34	0.33	0.68				
0.67	0.00	0.68					0.67	0.01	0.68					0.68	0.01	0.68				
0.34	0.17	0.62					0.34	0.17	0.62					0.34	0.17	0.62				
0.67	0.84	0.62					0.67	0.84	0.62					0.67	0.83	0.62				
0.01	0.50	0.62					0.01	0.50	0.62					0.01	0.50	0.62				
0.17	0.83	0.62					0.17	0.84	0.62					0.17	0.83	0.62				
0.51	0.50	0.62					0.51	0.50	0.62					0.51	0.50	0.62				
0.84	0.17	0.62					0.84	0.17	0.62					0.84	0.17	0.62				
0.17	0.34	0.62					0.17	0.34	0.62					0.17	0.33	0.62				
0.51	0.00	0.62					0.51	0.00	0.62					0.51	1.00	0.62				
0.84	0.67	0.62					0.84	0.67	0.62					0.84	0.67	0.62				
0.01	0.00	0.62					0.01	0.00	0.62					0.01	0.00	0.62				
0.34	0.67	0.62					0.34	0.67	0.62					0.34	0.67	0.62				
0.67	0.33	0.62					0.67	0.33	0.62					0.67	0.33	0.62				

0.50	0.50	0.72
0.37	0.50	0.78
0.33	0.41	0.81
0.62	0.52	0.79
0.59	0.44	0.82
0.64	0.47	0.86
0.50	0.33	0.82

0.50	0.50	0.73
0.40	0.51	0.78
0.47	0.54	0.83
0.64	0.43	0.79
0.62	0.43	0.83
0.69	0.44	0.86
0.44	0.44	0.84

0.52	0.50	0.73
0.38	0.48	0.78
0.36	0.39	0.82
0.66	0.55	0.79
0.64	0.49	0.82
0.53	0.40	0.83
0.36	0.44	0.84

(d)

10.96	0.00	0.00			
-5.49	9.51	0.00			
-0.08	0.20	26.31			
S	Mo	Ni	O	C	H
24	12	1	3	1	2
Direct					
0.17	0.50	0.56			
0.51	0.17	0.56			
0.84	0.84	0.56			
0.17	0.00	0.56			
0.51	0.67	0.56			
0.84	0.34	0.56			
0.01	0.17	0.56			
0.34	0.84	0.56			
0.67	0.50	0.56			
0.17	0.50	0.68			
0.50	0.16	0.68			
0.84	0.83	0.68			
0.17	1.00	0.68			
0.51	0.67	0.68			
0.84	0.33	0.68			
0.01	0.17	0.68			
0.34	0.83	0.68			
0.68	0.50	0.68			
0.00	0.67	0.56			
0.34	0.34	0.56			
0.67	0.00	0.56			
0.01	0.67	0.68			
0.33	0.33	0.68			
0.67	0.00	0.68			
0.34	0.17	0.62			
0.67	0.84	0.62			
0.01	0.50	0.62			
0.17	0.83	0.62			
0.51	0.50	0.62			
0.84	0.17	0.62			

(e)

10.96	0.01	0.00			
-5.49	9.50	0.00			
0.03	-0.03	26.53			
S	Mo	Ni	O	C	H
24	12	1	3	1	2
Direct					
0.17	0.50	0.56			
0.51	0.17	0.56			
0.84	0.84	0.56			
0.17	0.00	0.56			
0.51	0.67	0.56			
0.84	0.34	0.56			
0.01	0.17	0.56			
0.34	0.84	0.56			
0.67	0.50	0.56			
0.17	0.50	0.68			
0.50	0.17	0.68			
0.84	0.84	0.68			
0.17	0.00	0.68			
0.51	0.68	0.68			
0.84	0.34	0.68			
0.00	0.17	0.68			
0.34	0.84	0.68			
0.68	0.50	0.68			
0.00	0.67	0.56			
0.34	0.34	0.56			
0.67	0.00	0.56			
0.01	0.67	0.68			
0.33	0.33	0.68			
0.67	0.00	0.68			
0.34	0.17	0.62			
0.67	0.84	0.62			
0.00	0.50	0.62			
0.17	0.84	0.62			
0.51	0.50	0.62			
0.84	0.17	0.62			

(f)

10.95	0.00	0.00			
-5.48	9.52	0.00			
0.03	-0.01	26.59			
S	Mo	Ni	O	C	H
24	12	1	3	1	2
Direct					
0.17	0.50	0.56			
0.50	0.17	0.56			
0.84	0.84	0.56			
0.17	0.00	0.56			
0.50	0.67	0.56			
0.84	0.34	0.56			
0.00	0.17	0.56			
0.34	0.84	0.56			
0.67	0.50	0.56			
0.17	0.50	0.68			
0.50	0.17	0.68			
0.84	0.84	0.68			
0.17	0.00	0.68			
0.50	0.67	0.68			
0.84	0.33	0.68			
0.00	0.17	0.68			
0.34	0.84	0.68			
0.67	0.50	0.68			
0.00	0.67	0.56			
0.34	0.34	0.56			
0.67	0.00	0.56			
0.00	0.67	0.68			
0.33	0.33	0.68			
0.67	0.00	0.68			
0.34	0.17	0.62			
0.67	0.84	0.62			
0.00	0.50	0.62			
0.17	0.84	0.62			
0.50	0.50	0.62			
0.84	0.17	0.62			

0.17	0.33	0.62
0.51	0.00	0.62
0.84	0.67	0.62
0.01	0.00	0.62
0.34	0.67	0.62
0.67	0.33	0.62
0.51	0.50	0.72
0.38	0.50	0.77
0.38	0.45	0.82
0.64	0.58	0.79
0.61	0.52	0.83
0.56	0.41	0.84
0.37	0.52	0.84

0.17	0.34	0.62
0.51	0.00	0.62
0.84	0.67	0.62
0.01	0.00	0.62
0.34	0.67	0.62
0.67	0.34	0.62
0.51	0.51	0.72
0.47	0.56	0.78
0.43	0.47	0.83
0.61	0.28	0.80
0.63	0.40	0.80
0.73	0.50	0.80
0.48	0.42	0.82

0.17	0.34	0.62
0.50	0.00	0.62
0.84	0.67	0.62
0.00	0.00	0.62
0.33	0.67	0.62
0.67	0.33	0.62
0.50	0.50	0.72
0.50	0.49	0.79
0.33	0.41	0.83
0.71	0.52	0.81
0.60	0.50	0.82
0.56	0.48	0.86
0.31	0.48	0.82

(g)

10.97	0.00	0.00			
-5.48	9.51	0.00			
0.00	-0.02	26.56			
S	Mo	Ni	O	C	H
24	12	1	3	1	2
Direct					
0.18	0.50	0.56			
0.51	0.17	0.56			
0.84	0.84	0.56			
0.17	0.00	0.56			
0.51	0.67	0.56			
0.84	0.34	0.56			
0.01	0.17	0.56			
0.34	0.83	0.56			
0.67	0.50	0.56			
0.17	0.50	0.68			
0.51	0.17	0.68			
0.84	0.84	0.68			
0.17	0.00	0.68			
0.51	0.67	0.68			
0.84	0.34	0.68			
0.01	0.17	0.68			
0.34	0.84	0.68			
0.68	0.50	0.68			
0.01	0.67	0.56			
0.34	0.34	0.56			
0.67	0.00	0.56			
0.01	0.67	0.68			
0.33	0.33	0.68			

(h)

10.95	0.00	0.00			
-5.49	9.50	0.00			
0.01	-0.01	26.57			
S	Mo	Ni	O	C	H
24	12	1	3	1	2
Direct					
0.17	0.50	0.56			
0.51	0.17	0.56			
0.84	0.84	0.56			
0.17	0.00	0.56			
0.51	0.67	0.56			
0.84	0.33	0.56			
0.01	0.17	0.56			
0.34	0.83	0.56			
0.67	0.50	0.56			
0.17	0.50	0.68			
0.51	0.17	0.68			
0.84	0.84	0.68			
0.17	0.00	0.68			
0.51	0.67	0.68			
0.84	0.33	0.68			
0.01	0.17	0.68			
0.34	0.84	0.68			
0.67	0.50	0.68			
0.00	0.67	0.56			
0.34	0.34	0.56			
0.67	0.00	0.56			
0.01	0.67	0.68			
0.34	0.33	0.68			

(i)

10.97	0.00	0.00			
-5.45	9.52	0.00			
0.00	0.06	26.64			
S	Mo	Ni	O	C	H
24	12	1	3	1	2
Direct					
0.17	0.50	0.56			
0.51	0.17	0.56			
0.84	0.84	0.56			
0.17	0.00	0.56			
0.51	0.67	0.56			
0.84	0.34	0.56			
0.01	0.17	0.56			
0.34	0.83	0.56			
0.67	0.50	0.56			
0.17	0.50	0.68			
0.51	0.17	0.68			
0.84	0.84	0.68			
0.17	0.00	0.68			
0.50	0.67	0.68			
0.84	0.34	0.68			
0.01	0.17	0.68			
0.34	0.84	0.68			
0.67	0.50	0.68			
0.01	0.67	0.56			
0.34	0.34	0.56			
0.67	0.00	0.56			
0.01	0.67	0.68			
0.34	0.33	0.68			

0.68	0.00	0.68
0.34	0.17	0.62
0.68	0.84	0.62
0.01	0.50	0.62
0.17	0.84	0.62
0.51	0.50	0.62
0.84	0.17	0.62
0.17	0.34	0.62
0.51	0.00	0.62
0.84	0.67	0.62
0.01	0.00	0.62
0.34	0.67	0.62
0.67	0.33	0.62
0.50	0.50	0.73
0.40	0.50	0.78
0.47	0.56	0.82
0.60	0.41	0.78
0.61	0.43	0.83
0.68	0.41	0.85
0.43	0.48	0.85

0.67	0.00	0.68
0.34	0.17	0.62
0.67	0.84	0.62
0.01	0.50	0.62
0.17	0.83	0.62
0.51	0.50	0.62
0.84	0.17	0.62
0.17	0.34	0.62
0.51	0.00	0.62
0.84	0.67	0.62
0.01	0.00	0.62
0.34	0.67	0.62
0.67	0.33	0.62
0.50	0.48	0.73
0.36	0.46	0.77
0.59	0.56	0.87
0.64	0.56	0.78
0.61	0.51	0.83
0.63	0.42	0.83
0.41	0.51	0.80

0.67	0.01	0.68
0.34	0.17	0.62
0.67	0.84	0.62
0.01	0.50	0.62
0.17	0.84	0.62
0.51	0.50	0.62
0.84	0.17	0.62
0.17	0.34	0.62
0.51	0.00	0.62
0.84	0.67	0.62
0.01	0.00	0.62
0.34	0.67	0.62
0.67	0.33	0.62
0.51	0.50	0.72
0.48	0.49	0.79
0.75	0.56	0.85
0.79	0.76	0.81
0.77	0.66	0.83
0.44	0.40	0.81
0.41	0.52	0.80