

**Enhanced sensing characteristics of N doped and (N, O) co-doped molybdenum
disulfide to detect toxic gases: A comprehensive first-principles study**

*Khiet An Vuong¹, Nguyen Hai Dang², Le Phuong Truong³, Pham Minh Thuan⁴, D.M. Hoat^{5,6},
Minh Triet Dang⁷, Guo-Ping Chang-Chien⁴, Duy Khanh Nguyen^{8,9,*}*

¹College of Natural Sciences, Can Tho University, Can Tho City, Vietnam

²Faculty of Basic Sciences, Nam Can Tho University, Can Tho City, Viet Nam

³Faculty of Mechatronics and Electronics, Lac Hong University, Dong Nai Province, Vietnam

*⁴Center for Environmental Toxin and Emerging-Contaminant Research, Cheng Shiu University,
Kaohsiung City, Taiwan*

⁵Institute of Theoretical and Applied Research, Duy Tan University, Ha Noi 100000, Vietnam

⁶School of Engineering and Technology, Duy Tan University, Da Nang 550000, Vietnam

⁷School of Education, Can Tho University, Can Tho City, Vietnam

*⁸Laboratory for Computational Physics, Institute for Computational Science and Artificial
Intelligence, Van Lang University, Ho Chi Minh City, Vietnam*

*⁹Faculty of Mechanical, Electrical, and Computer Engineering, Van Lang School of Technology,
Van Lang University, Ho Chi Minh City, Vietnam*

**Corresponding author: Duy Khanh Nguyen (khanh.nguyenduy@vlu.edu.vn)*

Table S1. Dependence of the work function values (eV) on different k-point meshes with a fixed ENCUT of 500 eV for the MoS₂, N-MoS₂, and N-O-MoS₂ before and after adsorption of CO, CO₂, and NH₃ gases.

k-point meshes	MoS ₂				N-MoS ₂				N-O-MoS ₂			
	pristine	CO	CO ₂	NH ₃	substrate	CO	CO ₂	NH ₃	substrate	CO	CO ₂	NH ₃
5x5x1	5.525	5.637	6.584	5.701	5.648	5.508	5.615	5.642	6.640	5.570	5.650	6.104
7x7x1	5.514	5.640	6.548	5.689	5.643	5.519	5.611	5.620	6.622	5.542	5.626	6.157
9x9x1	5.516	5.648	6.567	5.683	5.630	5.536	5.628	5.617	6.620	5.544	5.625	6.171
11x11x1	5.515	5.615	6.563	5.688	5.624	5.520	5.612	5.621	6.626	5.550	5.630	6.167
variation	0.001	0.003	0.017	0.012	0.005	0.011	0.004	0.021	0.02	0.02	0.02	0.053
	-	-	-	-	-	-	-	-	-	-	-	-
	0.011	0.022	0.021	0.018	0.024	0.028	0.013	0.025	0.018	0.028	0.025	0.067

Table S2. Dependence of the E_{ads} (eV) on different k-point meshes of the MoS₂-CO configuration with a fixed ENCUT of 500 eV.

k-point meshes	E _{ads}
5x5x1	-0.151001
7x7x1	-0.151000
9x9x1	-0.151002
11x11x1	-0.151003
variation	0.000001 - 0.000002

Table S3. Dependence of the work function values (eV) on different ENCUT values with the fixed k-point mesh of 5x5x1 for the MoS₂, N-MoS₂, and N-O-MoS₂ before and after adsorption of CO, CO₂, and NH₃ gases.

ENCUT values	MoS ₂				N-MoS ₂				N-O-MoS ₂			
	pristine	CO	CO ₂	NH ₃	substrate	CO	CO ₂	NH ₃	substrate	CO	CO ₂	NH ₃
500	5.525	5.637	6.584	5.701	5.648	5.508	5.615	5.642	6.640	5.570	5.650	6.104
550	5.531	5.654	6.584	5.710	5.655	5.511	5.643	5.632	6.656	5.548	5.651	6.106
600	5.535	5.647	6.584	5.722	5.656	5.511	5.643	5.632	6.656	5.548	5.651	6.107
650	5.540	5.657	6.585	5.706	5.655	5.511	5.643	5.632	6.656	5.548	5.651	6.107
variation	0.006	0.01		0.005	0.007							0.002
	-	-	0.001	-	-	0.003	0.028	0.01	0.0016	0.022	0.001	-
	0.015	0.02		0.021	0.008							0.003

Table S4. Dependence of the E_{ads} (eV) on different ENCUT values of the MoS₂-CO configuration with the fixed k-point mesh of 5x5x1.

ENCUT values	E _{ads}
500	-0.15001
550	-0.15004
600	-0.15004
650	-0.15004
Variation	0.00003

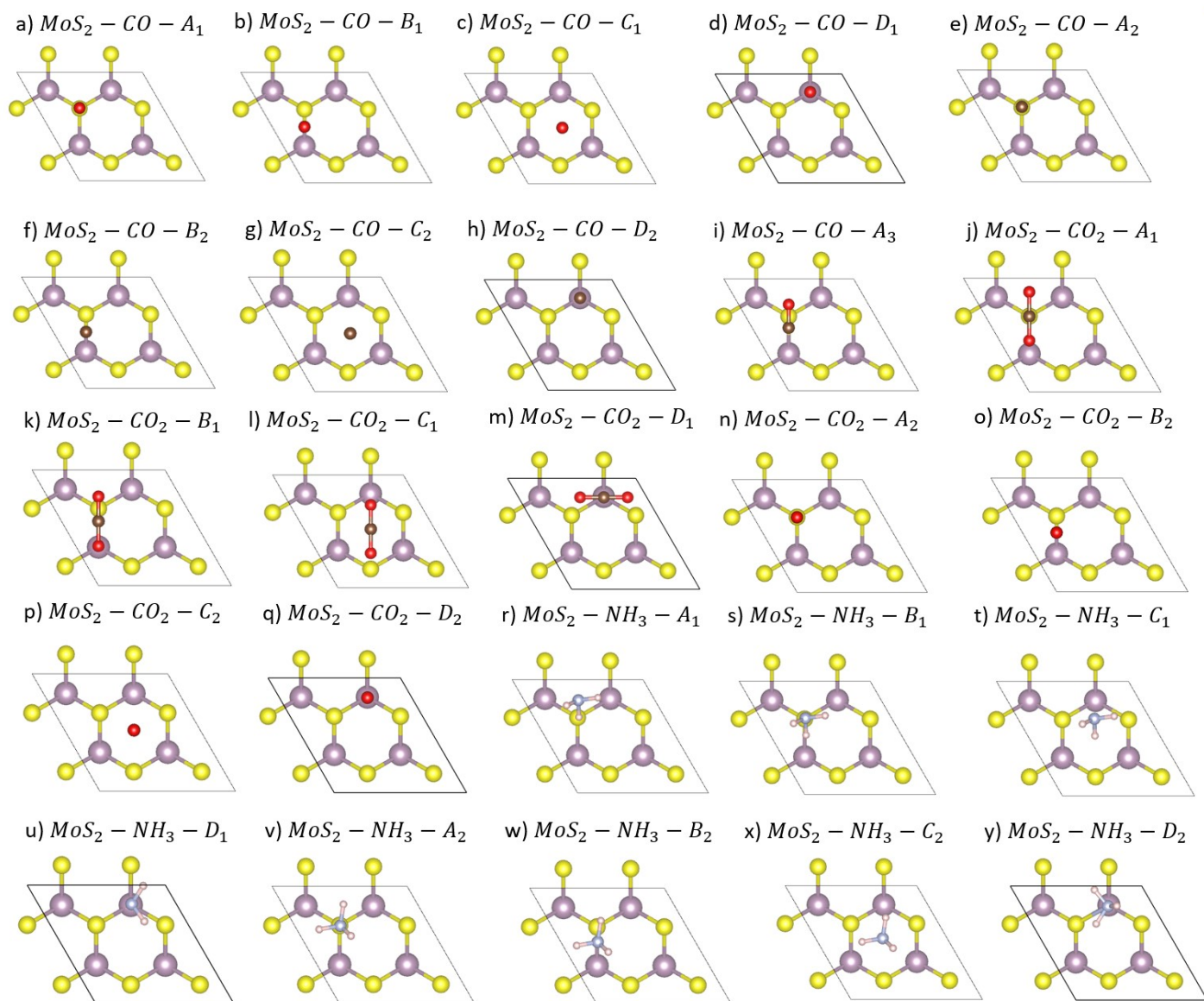


Figure S1. 25 possible (initial) adsorption configurations of the pristine MoS_2 for CO (a-i), CO_2 (j-q), and NH_3 (r-y).

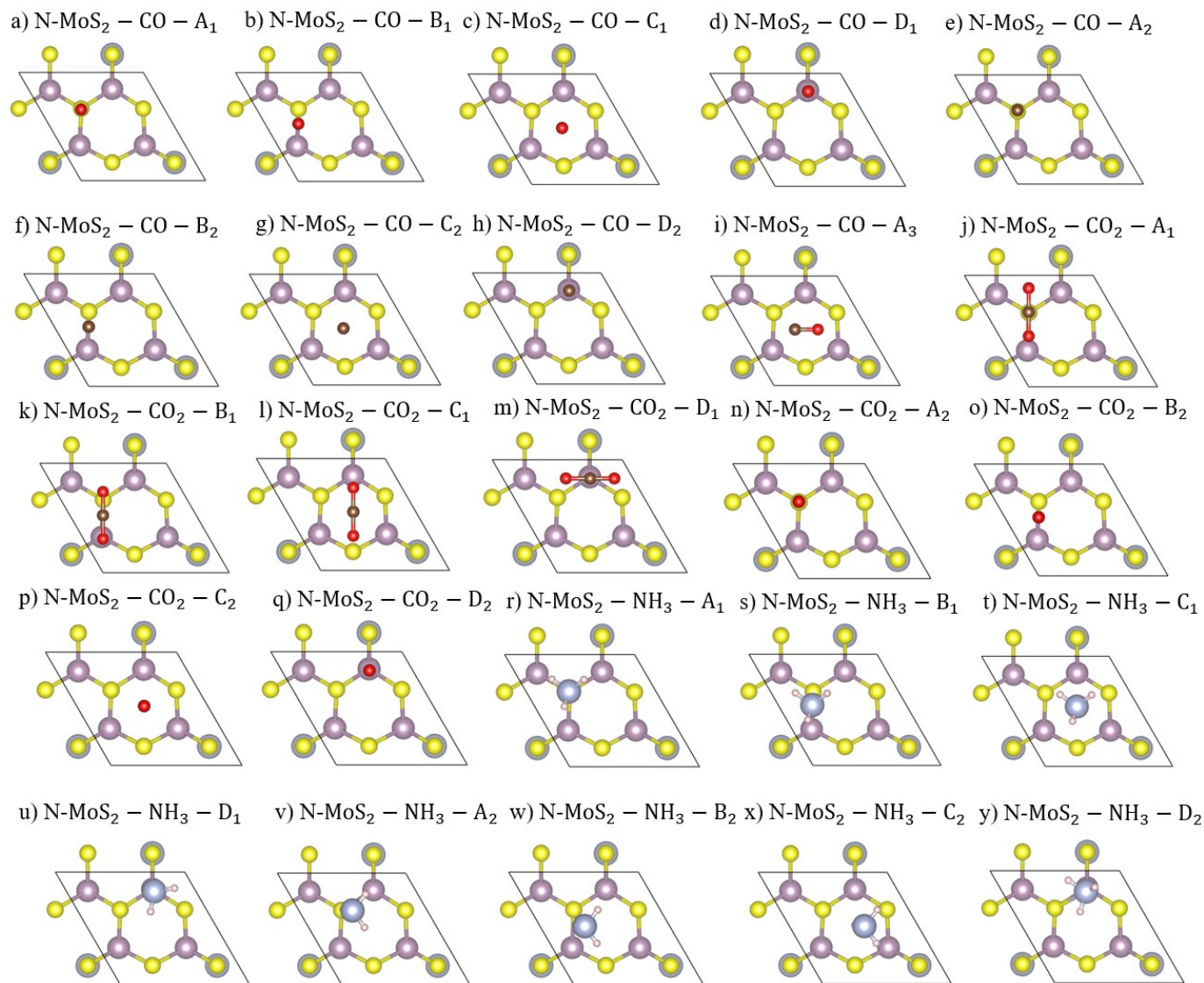


Figure S2. 25 possible (initial) adsorption configurations of N doped MoS₂ for CO (a-i), CO₂ (j-q), and NH₃ (r-y).

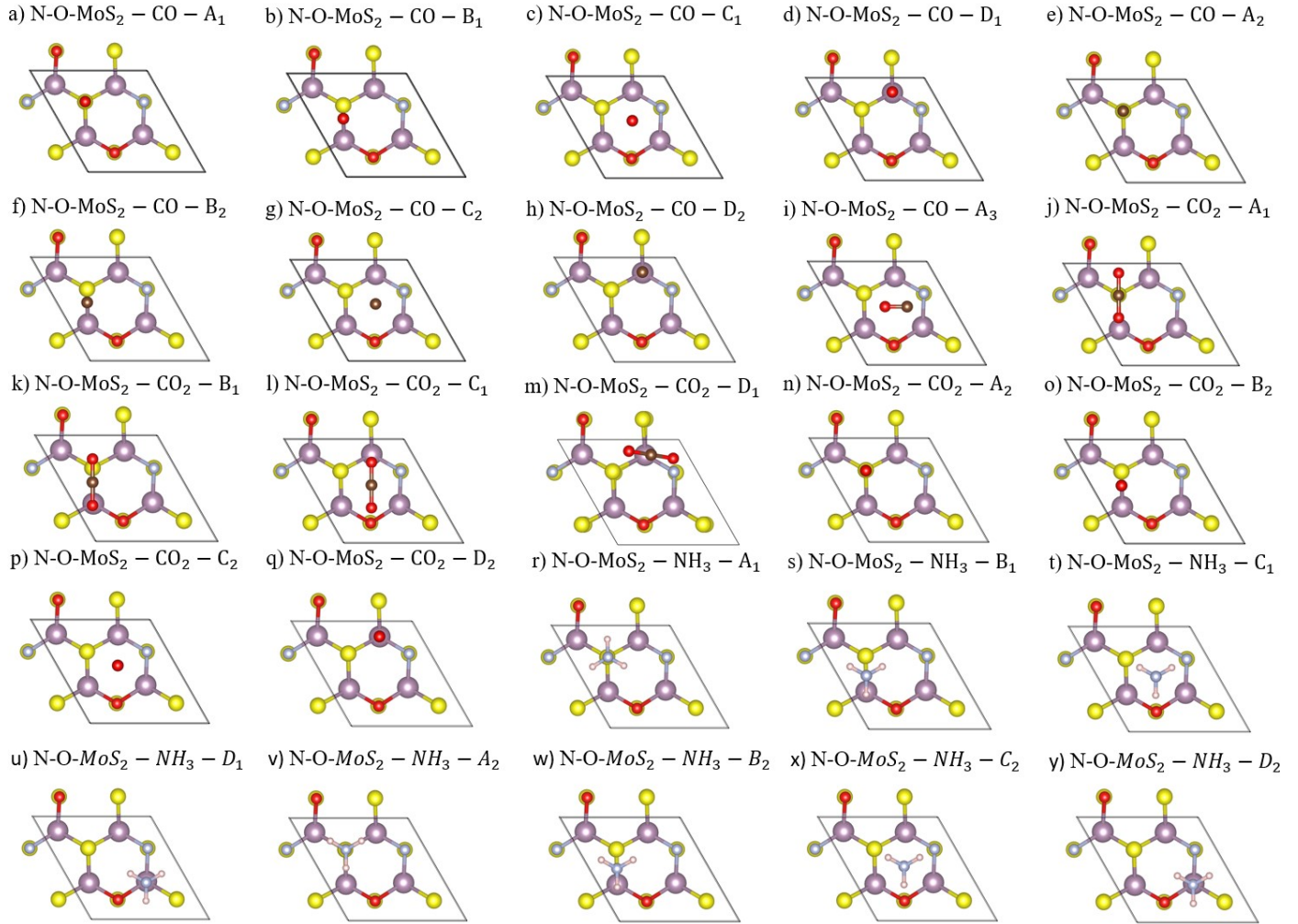


Figure S3. 25 possible (initial) adsorption configurations of (N, O) co-doped-MoS₂ for CO (a-i),

CO₂ (j-q), and NH₃ (r-y).

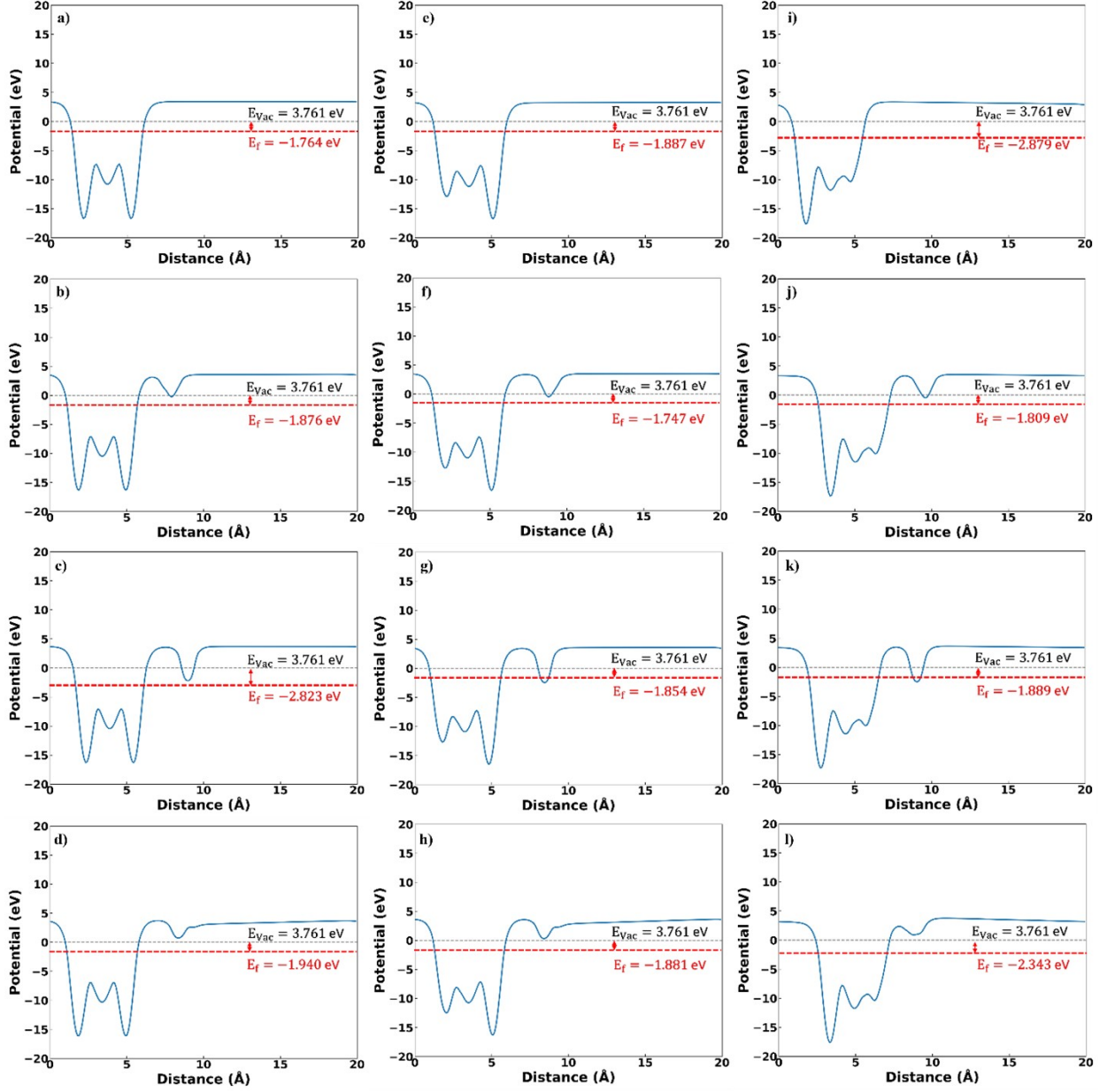


Figure S4. The ϕ along the z-direction of (a) pristine-MoS₂, (b) MoS₂-CO-B₁, (c) MoS₂-CO₂-A₁, (d) MoS₂-NH₃-A₁, (e) N-MoS₂, (f) N-MoS₂-CO-D₁, (g) N-MoS₂-CO₂-A₁, (h) N-MoS₂-NH₃-A₁, (i) N-O-MoS₂, (j) N-O-MoS₂-CO-D₁, (k) N-O-MoS₂-CO₂-D₁, (l) N-O-MoS₂-NH₃-D₁, whereas the vacuum level (E_{vac}) and Fermi level (E_f) are illustrated by solid blue and dashed red lines, respectively.