Selective sensing characteristics of Fe doped and (Fe, N, O) co-doped molybdenum disulfide toward CO, CO_2, and NH_3 gases: A first–principles investigation

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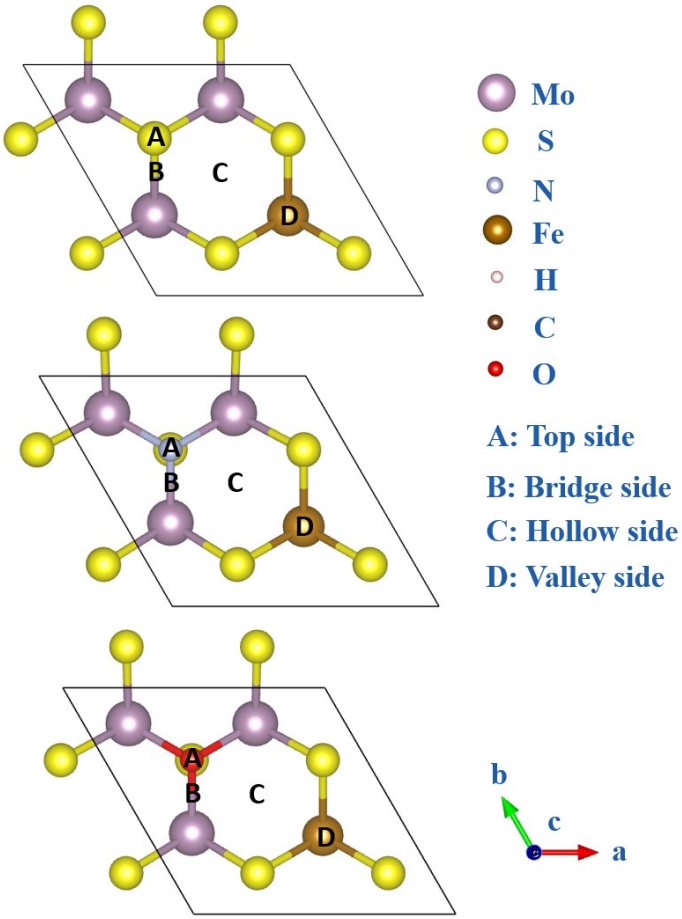

Figure S1. The 4 possible adsorption sites of CO, CO_2, and NH_3 gases on the doped/co-doped MoS_2 systems are considered, including four positions: A (on top of S), B (Mo–S bridge), C (center of the MoS_2 hexagon), and D (on top of Mo).

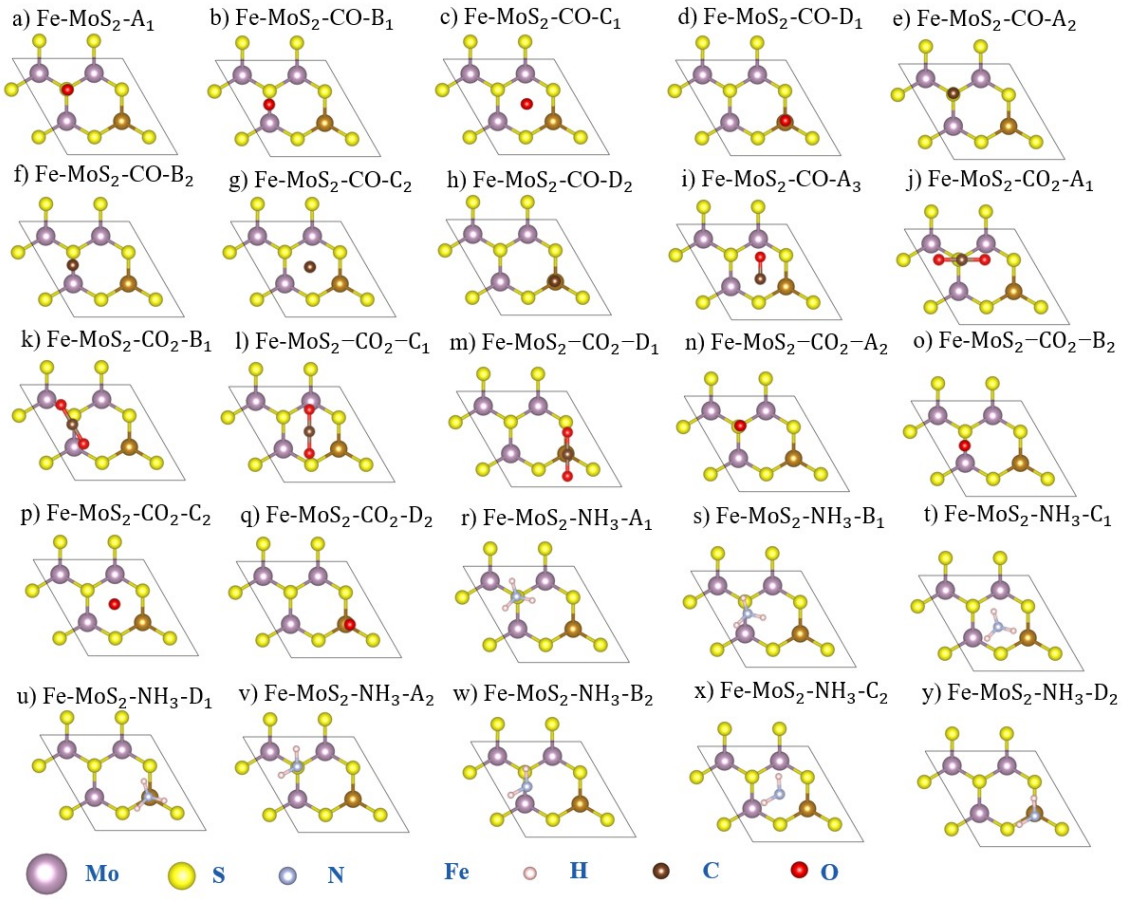

Figure S2. 25 possible (initial) adsorption configurations of the Fe–MoS_2 for CO (a-i), CO_2 (j-q), and NH_3 (r-y).

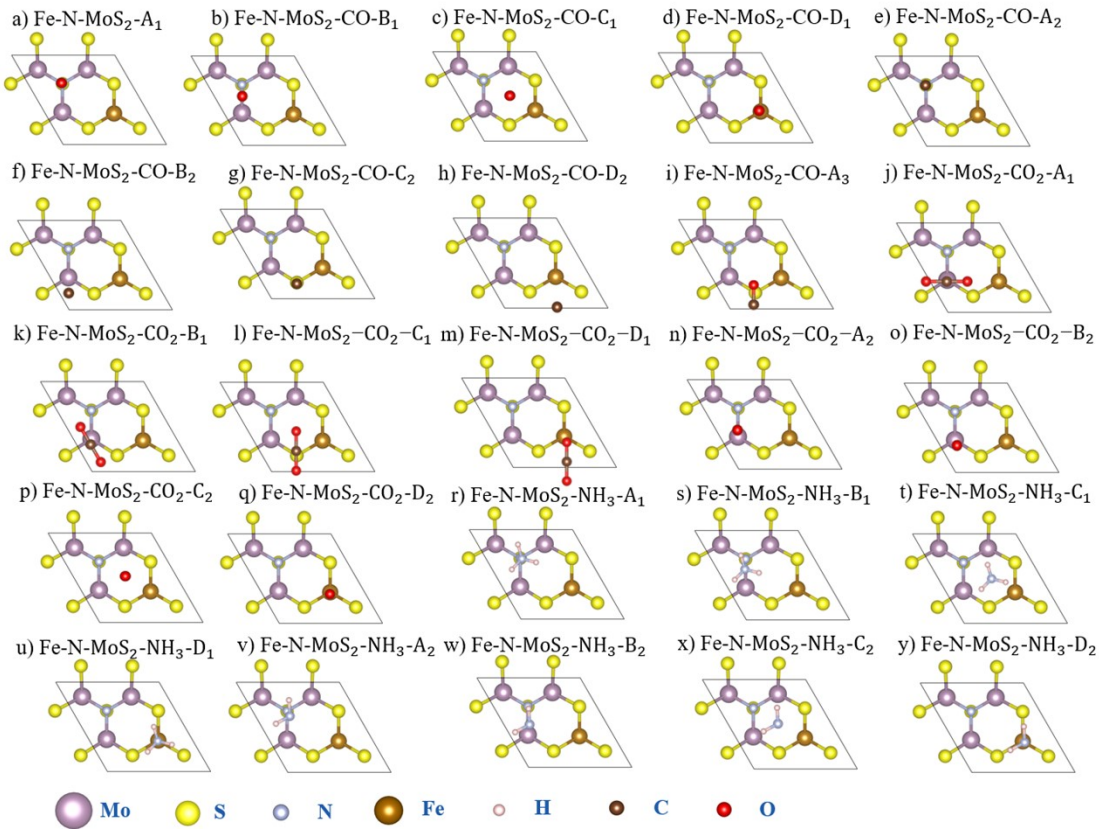

Figure S3. 25 possible (initial) adsorption configurations of Fe–N–MoS_2 for CO (a-i), CO_2 (j-q), and NH_3 (r-y).

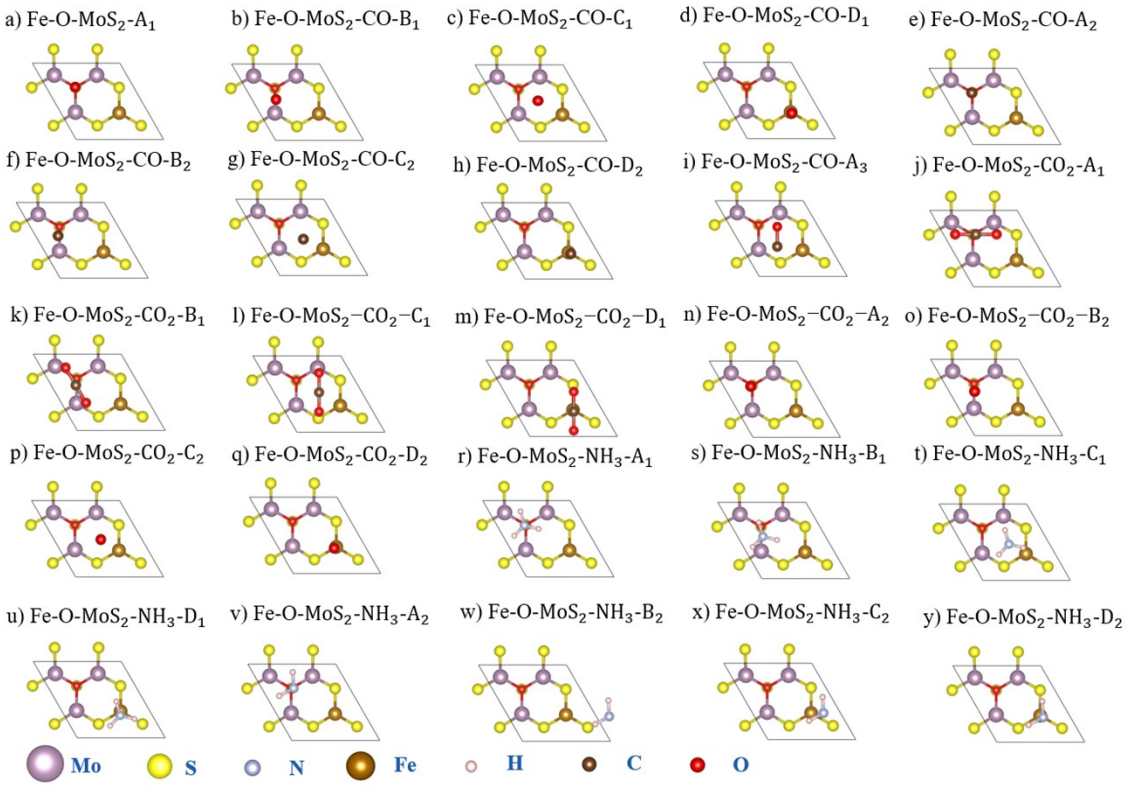

Figure S4. 25 possible (initial) adsorption configurations of Fe–O–MoS_2 for CO (a-i), CO_2 (j-q), and NH_3 (r-y).