Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Noble Metal (Ag, Au, Pd and Pt) Doped TaS_2 Monolayer for Gas Sensing: A First-Principle Investigation

Jia Shi, Wenjing Quan, Xinwei Chen, Xiyu Chen, Yongwei Zhang, Wen Lv, Jianhua Yang*, Min Zeng*, Hao Wei, Nantao Hu, Yanjie Su, Zhihua Zhou, Zhi Yang*

Key Laboratory of Thin Film and Microfabrication (Ministry of Education), Department of Micro/Nano Electronics, School of Electronic Information and Electrical Engineering, Institute of Marine Equipment, Shanghai Jiao Tong University, Shanghai 200240, P. R. China.

*Corresponding authors. E-mail address: yangjh08@sjtu.edu.cn (J. H. Yang), minzeng@sjtu.edu.cn (M. Zeng), zhiyang@sjtu.edu.cn (Z. Yang)

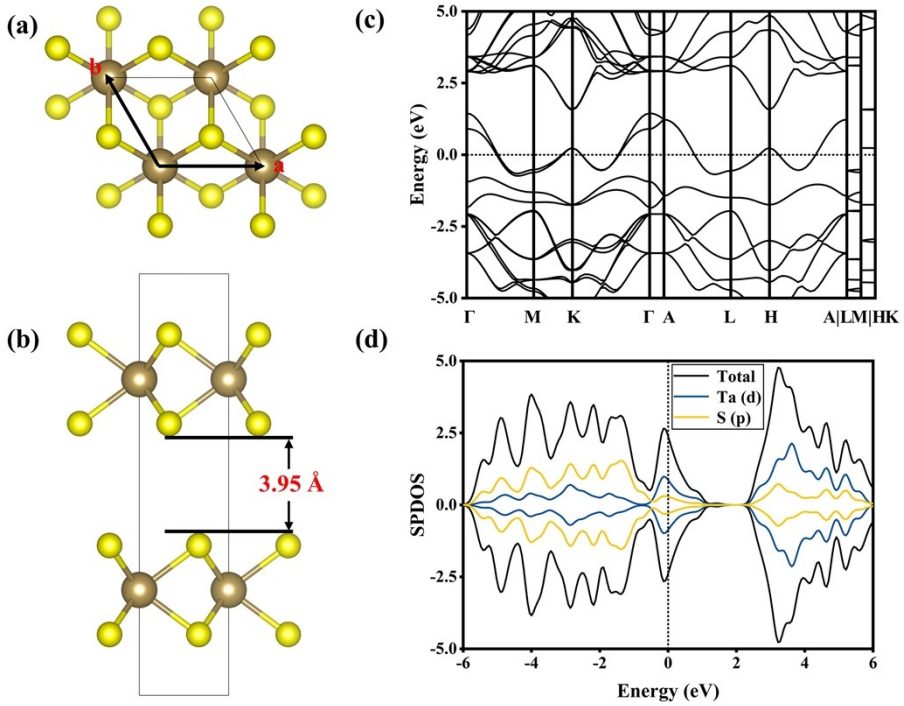


Fig. S1 Schematic of the primitive cell of the bulk TaS_2 (a, b), the band structure (c), and the spin-polarized projected density of states (d).

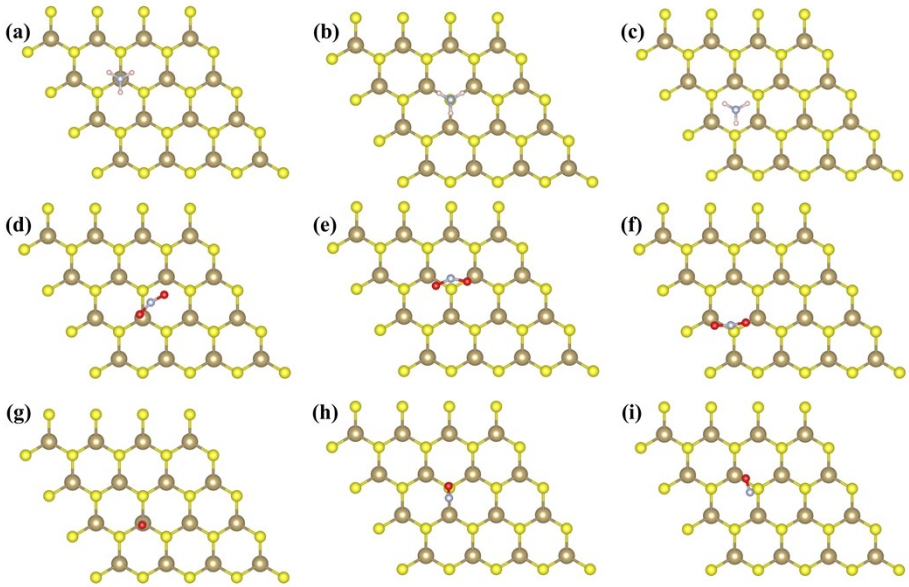


Fig. S2 Possible adsorption configuration of NH_3 (a, b, c), NO_2 (d, e, f), and NO (g, h, i) adsorbed on the TaS_2 monolayer.

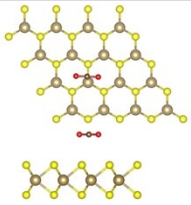
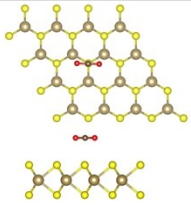
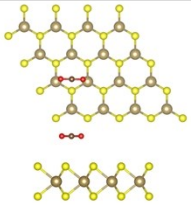
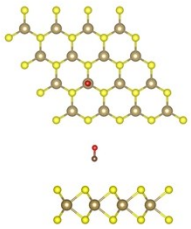
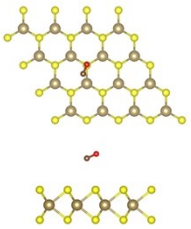
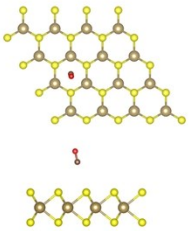
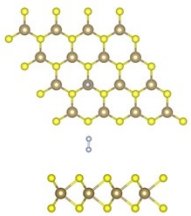
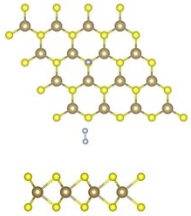
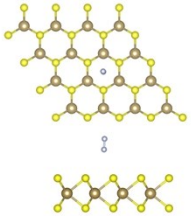
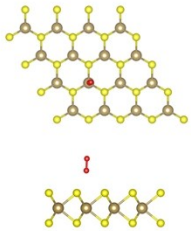
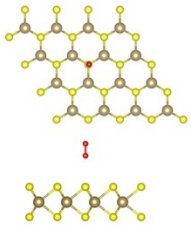
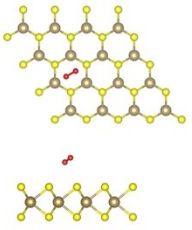
	T_{Ta} site	T_S site	H site
CO_2	 E_{ads} = -0.24 eV Q_T = 0.017 e	 E_{ads} = -0.13 eV Q_T = 0.028 e	 E_{ads} = -0.24 eV Q_T = 0.016 e
CO	 E_{ads} = -0.15 eV Q_T = 0.001 e	 E_{ads} = -0.16 eV Q_T = 0.007 e	 E_{ads} = -0.15 eV Q_T = 0.001 e
N_2	 E_{ads} = -0.14 eV Q_T = 0.008 e	 E_{ads} = -0.13 eV Q_T = 0.007 e	 E_{ads} = -0.14 eV Q_T = 0.009 e
O_2	 E_{ads} = -0.24 eV Q_T = 0.036 e	 E_{ads} = -0.12 eV Q_T = 0.027 e	 E_{ads} = -0.23 eV Q_T = 0.031 e

Fig. S3 Possible adsorption configurations of CO_2, CO, N_2 and O_2 adsorbed on TaS_2 monolayer.

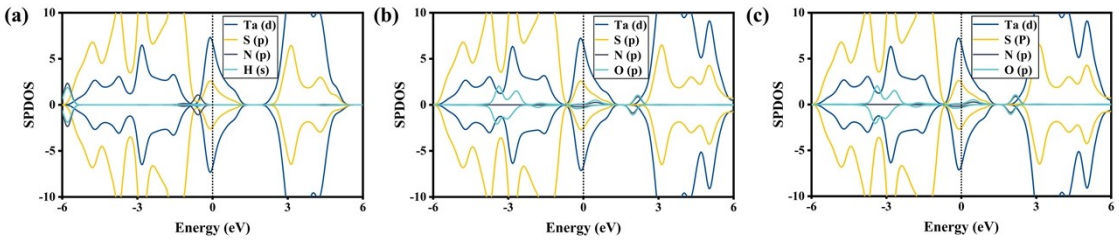


Fig. S4 The plots of spin-polarized projected density of states for the TaS_2 monolayer exposed to NH_3 (a), NO_2 (b) and NO (c), respectively.

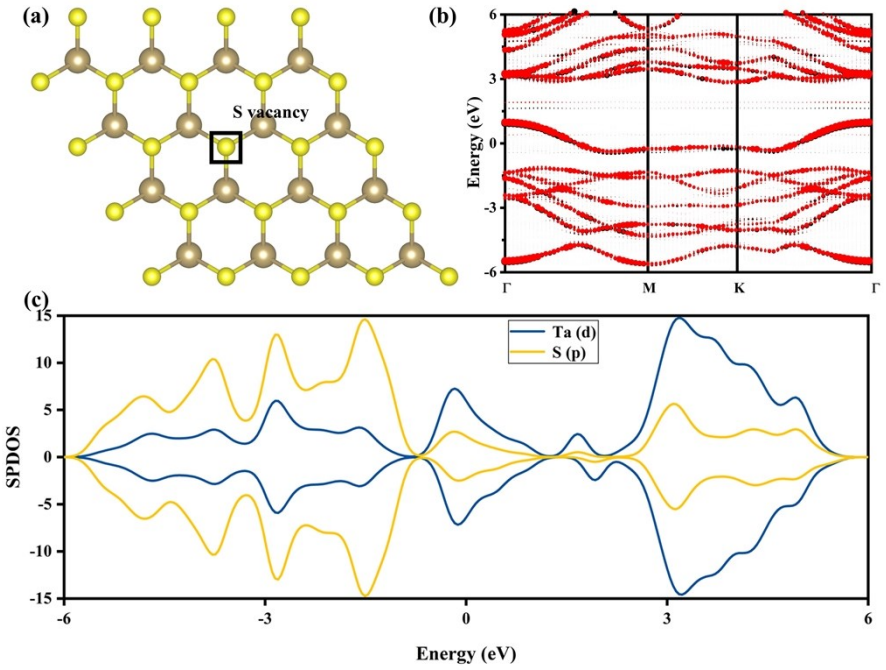


Fig. S5 A schematic diagram of a TaS_2 monolayer with a S vacancy (a), effective energy band (b), and spin-polarized projected density of states (c), respectively.

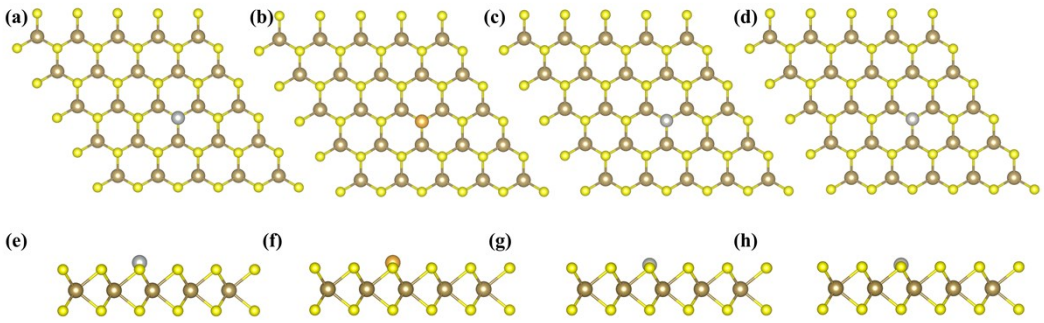


Fig. S6 Top view (a, b, c and d) and side view (e, f, g and h) of TaS_2 monolayer doped with noble metal atoms (Ag, Au, Pd and Pt, NM-doped TaS_2), respectively.

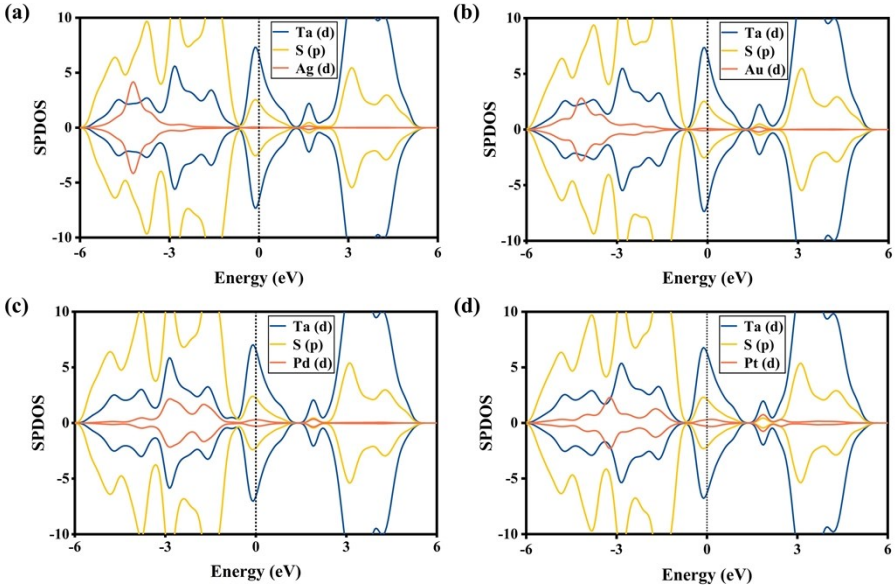


Fig. S7 The plots of spin-polarized projected density of states of NM-doped TaS_2 monolayer.

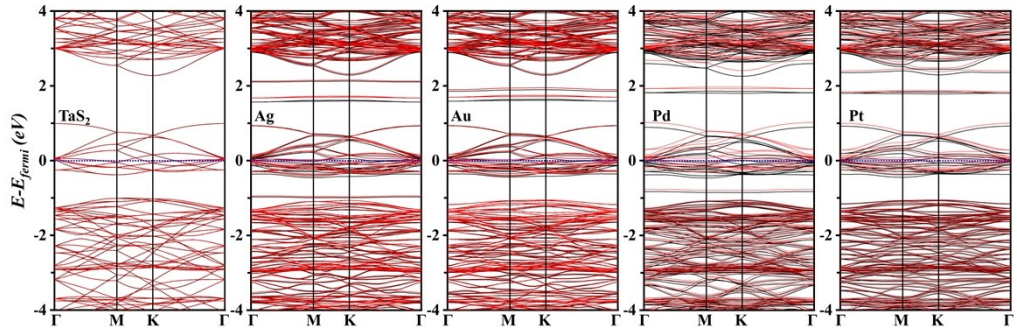


Fig. S8 Electronic band structures of intrinsic and NM-doped TaS_2. Black lines: spin up, red lines: spin down and the Fermi level is set to zero.

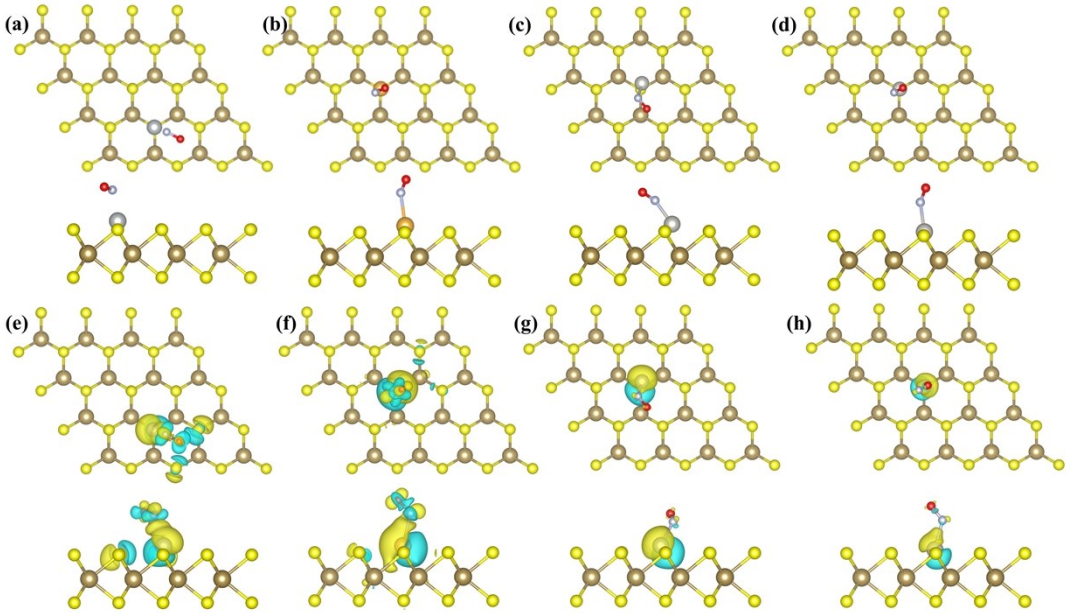


Fig. S9 The adsorption configuration (a, b, c and d) and the isosurface charge density plots (e, f, g and h) of NO adsorbed on NM-doped TaS_2 monolayer using isovalue of 0.02 e/Å^3, respectively. Cyan: charge depletion. Yellow: charge accumulation.

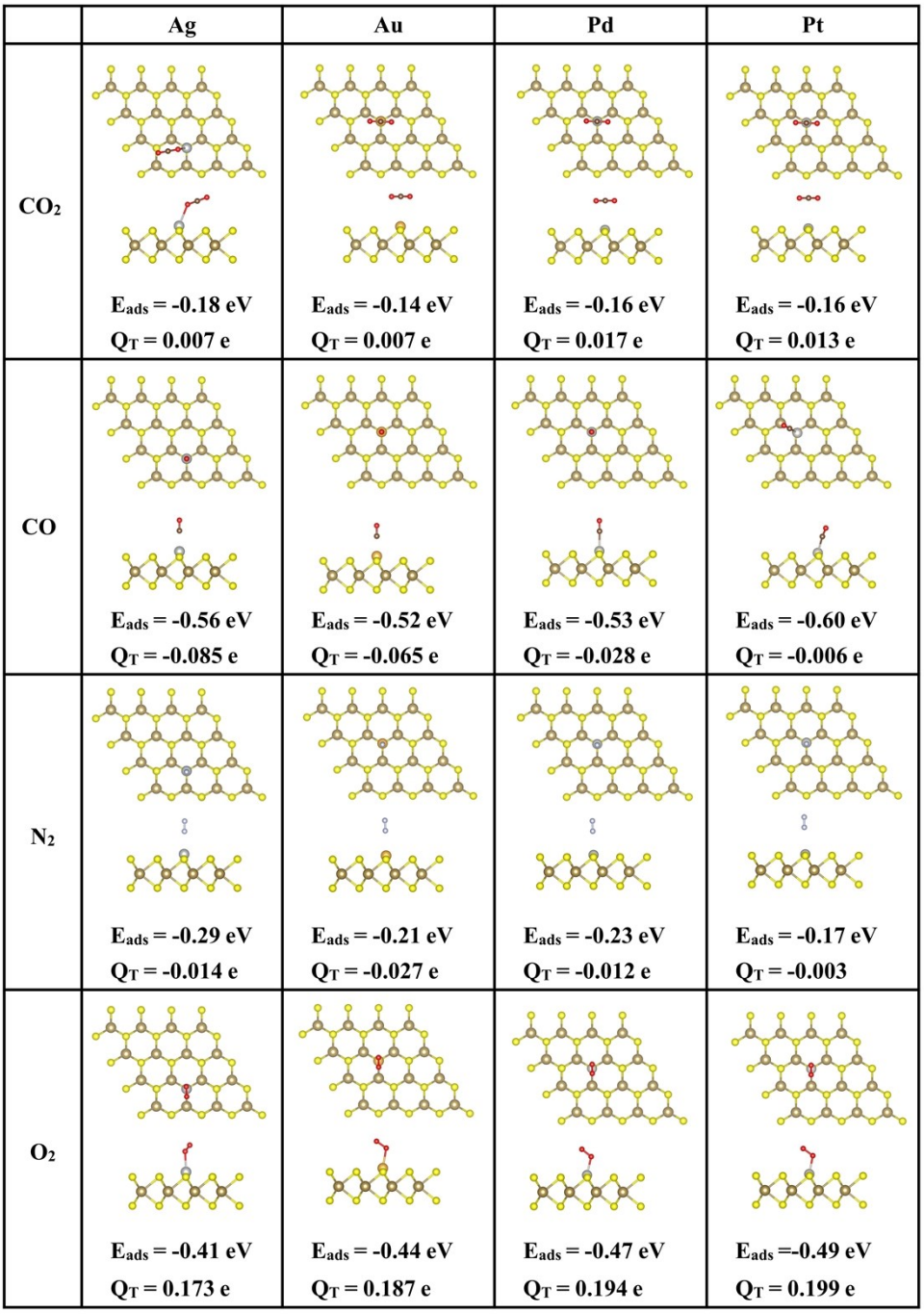


Fig. S10 Adsorption configurations of CO_2, CO, N_2 and O_2 adsorbed on NM-doped TaS_2 monolayer.

Table S1. The adsorption energy (E_{ads}), charge transfer (Q_T) and equilibrium height (h) of the system between gas molecule and TaS_2 monolayer.

Gas molecule	Sites	E_{ads} (eV)	Q_T (e)	h (Å)
NH_3	T_{Ta}	-0.2162	-0.0290	2.8849
	T_S	-0.2141	-0.0256	2.9460
	H	-0.2032	-0.0446	3.2459
NO_2	T_{Ta}	-0.3880	0.0430	2.4368
	T_S	-03904	0.0428	2.4329
	H	-0.3902	0.0439	2.4288
NO	T_{Ta}	-0.4902	-0.1741	1.9174
	T_S	-0.4409	-0.1707	2.3122
	H	-0.4472	-0.1709	2.3461

Table S2. The recovery time of the intrinsic and NM-doped TaS_2 monolayer exposed to NH_3, NO_2 and NO gas molecules.

System	Recovery time (s)		
	300 K	400 K	500 K
NH_3-TaS_2	4.26×10^{-9}	5.27×10^{-10}	1.51×10^{-10}
NH_3-Ag	2.49×10^{6}	62.7	1.09×10^{-1}
NH_3-Au	3.83×10^{5}	15.4	3.55×10^{-2}
NH_3-Pd	6.67×10^{3}	7.38×10^{-1}	3.12×10^{-3}
NH_3-Pt	8.39×10^{3}	8.77×10^{-1}	3.58×10^{-3}
NO-TaS_2	1.71×10^{-4}	1.49×10^{-6}	8.69×10^{-8}
NO-Ag	1.14×10^{-2}	3.50×10^{-5}	1.08×10^{-6}
NO-Au	1.07×10^{-1}	1.87×10^{-4}	4.14×10^{-6}
NO-Pd	9.82×10^{-1}	9.87×10^{-4}	1.57×10^{-5}
NO-Pt	2.17	1.79×10^{-3}	2.52×10^{-5}

NO_2-TaS_2	3.58×10^{-6}	8.22×10^{-8}	8.55×10^{-9}
NO_2-Ag	44.3	1.72×10^{-2}	1.54×10^{-4}
NO_2-Au	9.16×10^{2}	1.67×10^{-1}	9.49×10^{-4}
NO_2-Pd	2.62×10^{5}	11.6	2.82×10^{-2}
NO_2-Pt	8.62×10^{6}	1.59×10^{2}	2.30×10^{-1}