

## Electronic Supporting Information

# Heteroatom (Si, B, N, and P) doped 2D monolayer MoS<sub>2</sub> for NH<sub>3</sub> gas detection

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**Table S1. Global quantum descriptors (Ionization Potential, electron Affinity, chemical softness, chemical hardness, chemical potential, electrophilicity Index, and Femi level energy.**

Surfaces	IP	EA	$\sigma$	$\eta$	$\mu$	$\omega$	$E_{FL}$
B@MoS <sub>2</sub> QD	9.8067	6.4450	0.5949	1.6808	-8.1259	55.4930	8.1259
N@MoS <sub>2</sub> QD	9.7017	6.3261	0.5925	1.6878	-8.0139	54.1969	8.0139
P@MoS <sub>2</sub> QD	9.6369	6.2986	0.5991	1.6691	-7.9678	52.9832	7.9678
Si@MoS <sub>2</sub> QD	7.9806	3.6357	0.4603	2.1724	-5.8081	36.6427	5.8081
MoS <sub>2</sub> QD	7.1952	3.8847	-0.6041	1.6553	-5.5400	25.4011	5.5400
B@MoS <sub>2</sub> _NH <sub>3</sub>	9.8336	5.8753	0.2526	1.9791	-7.8544	15.5857	7.8544
B@MoS <sub>2</sub> _NH <sub>3</sub> -SP	8.3862	7.2420	0.8739	0.5721	-7.8141	53.3649	7.8141
B@MoS <sub>2</sub> _NH <sub>3</sub> -SP1	8.2181	7.2858	1.0727	0.4661	-7.7519	64.4625	7.7519
B@MoS <sub>2</sub> _NH <sub>3</sub> -SP2	9.2578	6.6131	0.3781	1.3223	-7.9354	23.8110	7.9354
N@MoS <sub>2</sub> _NH <sub>3</sub>	10.4652	5.8765	0.2179	2.2943	-8.1692	14.5438	8.1692
N@MoS <sub>2</sub> _NH <sub>3</sub> -SP	8.9253	7.3062	0.6176	0.8095	-8.1157	40.6822	8.1157
N@MoS <sub>2</sub> _NH <sub>3</sub> -SP1	8.7013	7.3625	0.7469	0.6694	-8.0319	48.1860	8.0319
N@MoS <sub>2</sub> _NH <sub>3</sub> -SP2	9.8328	6.7269	0.3219	1.5529	-8.2798	22.0732	8.2798
P@MoS <sub>2</sub> _NH <sub>3</sub>	9.7658	5.8548	0.2556	1.9555	-7.8103	15.5972	7.8103
P@MoS <sub>2</sub> _NH <sub>3</sub> -SP	8.7699	7.7859	1.1574	0.432	-8.2779	79.3097	8.2779
P@MoS <sub>2</sub> _NH <sub>3</sub> -SP2	9.5484	7.3470	0.4542	1.1007	-8.4477	32.4173	8.4477
Si@MoS <sub>2</sub> _NH <sub>3</sub>	7.7089	3.2465	0.2240	2.2312	-5.4777	7.7240	5.4777
Si@MoS <sub>2</sub> _NH <sub>3</sub> -SP	5.8626	4.9701	1.1205	0.4462	-5.4163	32.8734	5.4163
Si@MoS <sub>2</sub> _NH <sub>3</sub> -SP1	5.7203	5.0120	1.4120	0.3541	-5.3661	42.9316	5.3661
Si@MoS <sub>2</sub> _NH <sub>3</sub> -SP2	6.5753	4.4528	0.4733	1.0562	-5.5140	14.3932	5.5140
S@MoS <sub>2</sub> _NH <sub>3</sub>	7.4605	3.4626	0.2501	1.9989	-5.4615	7.4610	5.4615

S@MoS <sub>2</sub> NH <sub>3</sub> -SP	5.9628	4.8150	0.8712	0.5739	-5.3889	38.8342	5.3889
S@MoS <sub>2</sub> NH <sub>3</sub> -SP1	5.7995	4.8591	1.0633	0.4702	-5.3293	30.2014	5.3293
S@MoS <sub>2</sub> NH <sub>3</sub> -SP2	6.8795	4.1554	0.3671	1.3620	-5.5174	11.1753	5.5174

**Table S2:** Donor (i), Occupancy, Acceptor (j), Stabilization energies, Hybrid orbital and Atomic Orbital of the studied systems.

Surface	Donor (i)	Occupancy	Acceptor (i)	Occupancy	E(2)/Kcal/mol	E(j) – E(i)	F(j,i)	Hybrid	Atomic orbital
<b>B@MoS<sub>2</sub>_QD</b>	$\sigma\text{Mo}_1 - \text{B}_{36}$	1.37265	$\sigma^*\text{Mo}_1 - \text{Mo}_{13}$	0.53403	3836.88	0.09	0.525	spd <sup>41.99%</sup>	s(23.81) p(32.82%) d(43.37%)
	$\sigma\text{Mo}_1 - \text{B}_{36}$	1.37265	$\sigma^*\text{S}_3 - \text{M}_{04}$	0.29045	1238.31	0.02	0.161	spd <sup>41.99%</sup>	s(23.81) p(32.82%) d(43.37%)
	$\sigma\text{Mo}_1 - \text{B}_{36}$	1.37265	$\sigma^*\text{Mo}_1 - \text{S}_{11}$	0.21771	995.35	0.09	0.299	spd <sup>71.52%</sup>	s(12.02%) p(41.53%) d(46.45%)
	$\pi\text{Mo}_4 - \text{Mo}_5$	1.21786	$\sigma^*\text{Mo}_5 - \text{Mo}_{15}$	0.46915	1663.11	0.24	0.612	spd <sup>69.55%</sup>	s(7.61%) p(33.11%) d(59.28%)
	LP (1)Mo <sub>15</sub>	0.41943	$\sigma^*\text{Mo}_5 - \text{Mo}_{15}$	0.46915	5389.14	0.02	0.443	spd <sup>69.55%</sup>	s(7.61%) p(33.11%) d(59.28%)
	$\sigma^*\text{Mo}_1 - \text{S}_2$	0.16176	$\sigma\text{Mo}_1 - \text{B}_{36}$	1.37265	5180.34	0.02	0.340	spd <sup>41.99%</sup>	s(23.81) p(32.82%) d(43.37%)
	$\pi^*\text{Mo}_1 - \text{S}_3$	0.20751	$\sigma\text{Mo}_1 - \text{B}_{36}$	1.37265	2365.61	0.05	0.333	spd <sup>67.40%</sup>	s(0.19%) p(34.78%) d(65.03)
	$\sigma^*\text{Mo}_1 - \text{Mo}_{13}$	0.53403	$\sigma^*\text{Mo}_1 - \text{S}_9$	0.20065	1876.59	0.01	0.217	spd <sup>73.45%</sup>	s(13.75%) p(40.72%) d(45.53%)
	$\sigma^*\text{M}_{04} - \text{Mo}_5$	0.41840	$\pi^*\text{Mo}_4 - \text{Mo}_5$	0.41190	4098.73	0.04	0.568	spd <sup>44.96%</sup>	s(13.83%) p(26.23%) d(59.94)
	$\sigma\text{Mo}_4 - \text{Mo}_5$	1.46561	$\sigma^*\text{Mo}_5 - \text{Mo}_{15}$	0.46915	1347.51	0.07	0.412	spd <sup>66.59%</sup>	s(8.60%) p(2.80%) d(88.60%)
	$\pi^*\text{Mo}_4 - \text{Mo}_5$	0.41190	$\sigma^*\text{Mo}_5 - \text{Mo}_{15}$	0.46915	5797.69	0.03	0.553	spd <sup>66.59%</sup>	s(8.60%) p(2.80%) d(88.60%)
	$\sigma^*\text{Mo}_5 - \text{Mo}_6$	1.21786	$\sigma^*\text{Mo}_4 - \text{Mo}_5$	0.41840	2457.43	0.02	0.397	spd <sup>44.96%</sup>	s(13.83%) p(26.23%) d(59.94)
<b>N@MoS<sub>2</sub>_QD</b>	$\pi^*\text{Mo}_{20} - \text{S}_{28}$	0.68619	$\sigma\text{Mo}_{19} - \text{Mo}_{20}$	0.32692	410.29	0.02	0.082	spd <sup>49.03%</sup>	s(9.92%) p(36.66%) d(53.43%)
	$\sigma^*\text{M}_{019} - \text{S}_{27}$	0.16853	$\sigma^*\text{Mo}_{19} - \text{S}_{28}$	0.7865	191.68	0.01	0.107	spd <sup>61.85%</sup>	s(13.63%) p(34.11%) d(52.26%)
	$\sigma^*\text{Mo}_{18} - \text{S}_{34}$	0.21025	$\sigma^*\text{Mo}_{18} - \text{S}_{27}$	0.20236	757.20	0.01	0.17	spd <sup>72.63%</sup>	s(19.27%) p(41.60%) d(39.13%)
	$\sigma^*\text{Mo}_{18} - \text{S}_{34}$	0.21025	$\sigma^*\text{Mo}_{15} - \text{Mo}_{18}$	0.31210	405.44	0.05	0.249	Spd <sup>37.77</sup>	s(19.05%) p(14.97%) d(65.97%)
	$\sigma^*\text{Mo}_{18} - \text{S}_{31}$	0.20477	$\sigma^*\text{Mo}_{18} - \text{Mo}_{19}$	0.25756	448.14	0.02	0.188	spd <sup>67.90%</sup>	s(13.49%) p(0.90%) d(85.61%)
	$\sigma^*\text{M}_{018} - \text{S}_{27}$	0.20236	$\sigma^*\text{Mo}_{15} - \text{Mo}_{18}$	0.31210	484.59	0.04	0.243	spd <sup>37.77%</sup>	s(19.05%) p(14.97%) d(65.97%)
	$\sigma^*\text{Mo}_{14} - \text{S}_{30}$	0.22579	$\sigma^*\text{S}_{12} - \text{M}_{014}$	0.19580	332.11	0.02	0.138	spd <sup>38.57%</sup>	s(19.92%) p(79.89%) d(0.19%)
	$\sigma^*\text{Mo}_8 - \text{S}_{12}$	0.21025	$\sigma^*\text{Mo}_8 - \text{S}_{10}$	0.20236	757.20	0.01	0.175	spd <sup>72.63%</sup>	s(19.27%) p(41.60%) d(39.13%)
	$\sigma^*\text{Mo}_8 - \text{S}_{12}$	0.21025	$\sigma^*\text{Mo}_8 - \text{S}_{12}$	0.23843	405.44	0.01	0.175	Spd <sup>64.19%</sup>	s(2.58%) p(1.73%) d(95.69%)
	$\sigma^*\text{Mo}_8 - \text{S}_{10}$	0.20236	$\sigma^*\text{Mo}_8 - \text{M}_{013}$	0.31210	484.59	0.04	0.234	spd <sup>62.23%</sup>	s(17.27%) p(5.22%) d(77.51%)
	$\sigma^*\text{Mo}_8 - \text{S}_9$	0.20549	$\sigma^*\text{Mo}_8 - \text{Mo}_{14}$	0.27945	300.03	0.03	0.160	Spd <sup>72.00%</sup>	s(13.49%) p(0.90%) d(85.61%)
	$\sigma^*\text{M}_{05} - \text{S}_{24}$	0.19917	$\sigma^*\text{Mo}_5 - \text{Mo}_{15}$	0.35611	934.35	0.02	0.215	spd <sup>50.76%</sup>	s(25.11%) p(15.35%) d(59.54%)
	$\sigma^*\text{Mo}_5 - \text{Mo}_{15}$	0.35611	$\sigma^*\text{Mo}_5 - \text{S}_6$	0.21371	1591.04	0.01	0.251	Spd <sup>69.59%</sup>	s((10.89%)p(30.93%) d(58.18%)
	$\sigma^*\text{Mo}_{15} - \text{M}_{18}$	0.31210	$\sigma^*\text{Mo}_{18} - \text{Mo}_{19}$	0.257756	775.46	0.10	0.268	Spd <sup>67.90%</sup>	s(13.49%) p(0.90%) d(85.61%)
	$\sigma\text{Mo}_8 - \text{Mo}_{13}$	0.31210	$\sigma\text{Mo}_8 - \text{Mo}_{14}$	0.27945	966.99	0.07	0.254	spd <sup>72.00%</sup>	s(13.49%) p(0.90%) d(85.61)
	<b>P@MoS<sub>2</sub>_QD</b>	$\sigma^*\text{Mo}_{17} - \text{S}_{33}$	0.33451	$\sigma^*\text{Mo}_{17} - \text{Mo}_{20}$	0.35823	342.24	0.02	0.146	spd <sup>55.13%</sup>
$\sigma^*\text{Mo}_{14} - \text{S}_{30}$		0.23935	LP*Mo <sub>14</sub>	0.36994	312.11	0.03	0.155	spd	s(13.52%) p(78.27%) d(8.21%)
$\sigma^*\text{Mo}_{14} - \text{S}_{29}$		0.32049	LP*Mo <sub>14</sub>	0.36994	205.58	0.03	0.118	spd	s(13.52%) p(78.27%) d(8.21%)
$\sigma^*\text{Mo}_{14} - \text{S}_{23}$		0.35261	LP*Mo <sub>14</sub>	0.36994	266.74	0.04	0.174	spd	s(13.52%) p(78.27%) d(8.21%)

	$\sigma^*Mo_{14} - S_{22}$	0.31698	$LP^*Mo_{14}$	0.36994	332.32	0.02	0.121	Spd	s(13.52%) p(78.27%) d(8.21%)
	$\sigma^*Mo_8 - Mo_{14}$	0.36465	$\sigma^*Mo_8 - S_9$	0.18163	304.80	0.03	0.151	spd <sup>64.90%</sup>	s(16.55%) p(30.43%) d(53.02%)
	$\sigma^*Mo_8 - Mo_{14}$	0.36465	$\sigma^*Mo_8 - S_{11}$	0.18180	270.69	0.03	0.157	spd <sup>65.14</sup>	s(15.83%) p(31.94%) d(52.23%)
	$\sigma^*Mo_8 - S_{14}$	0.36465	$\sigma^*Mo_{14} - S_{29}$	0.32049	232.24	0.03	0.135	spd <sup>61.57%</sup>	s(9.02%) p(37.71%) d(53.27%)
	$\sigma^*Mo_5 - S_{31}$	0.25294	$\sigma^*Mo_5 - Mo_{15}$	0.42442	416.58	0.01	0.104	spd <sup>53.67%</sup>	s(28.01%) p(6.05%) d(65.94%)
	$\sigma^*Mo_4 - S_{21}$	0.24165	$\sigma^*Mo_{14} - S_{22}$	0.31698	228.66	0.02	0.135	spd <sup>61.79%</sup>	s(8.57%) p(39.16%) d(52.28%)
	$\sigma^*Mo_1 - Mo_{13}$	0.37352	$\sigma^*Mo_1 - S_3$	0.15584	583.69	0.02	0.193	spd <sup>57.74%</sup>	s(16.41%) p(13.56%) d(70.03%)
	$\sigma^*Mo_1 - Mo_{13}$	0.37352	$\sigma^*Mo_1 - S_3$	0.15584	454.73	0.03	0.193	spd <sup>57.74%</sup>	s(16.41%) p(13.56%) d(70.03%)
	$LP^*Mo_{16}$	0.38276	$LP^*Mo_{14}$	0.36994	655.03	0.02	0.149	spd	s(13.52%) p(78.27%) d(8.21%)
<b>Si@MoS<sub>2</sub>_QD</b>	$\pi^*Mo_{14} - S_{30}$	0.19163	$\pi^*Mo_{14} - S_{23}$	0.16096	1640.59	0.03	0.273	spd <sup>64.82%</sup>	s(14.91%) p(36.06%) d(49.03%)
	LP Si36	0.21354	$LP^*(2) Mo_{13}$	0.30269	1044.65	0.05	0.331	spd	s(0.12%) p(91.39%) d(8.49%)
	$\sigma Mo_8 - Mo_{13}$	0.44258	$\sigma Mo_8 - Mo_{14}$	0.24825	599.08	0.11	0.244	spd <sup>39.20%</sup>	s(7.18%) p(92.63%) d(0.19%)
	$LP^*Mo_{16}$	0.11019	$LP^*Mo_{20}$	0.11019	572.35	0.02	0.183	spd	S(0.78%) p(90.95%) d(8.28%)
	$\sigma^*Mo_1 - S_2$	0.19660	$\sigma^*Mo_1 - Mo_{13}$	0.46476	574.75	0.02	0.193	spd <sup>53.12%</sup>	s(26.73%) p(3.73%) d(69.54%)
	$\sigma^*Mo_8 - S_{12}$	0.28876	$\sigma^*Mo_8 - Mo_{13}$	0.44258	549.09	0.04	0.204	spd <sup>43.86%</sup>	s(17.80%) p(4.47%) d(77.73%)
	$\sigma^*Mo_{19} - S_{27}$	0.24825	$\sigma^*Mo_{19} - S_{28}$	0.16096	553.35	0.01	0.148	spd <sup>64.82%</sup>	s(14.91%) p(36.06%) d(49.03%)
	$LP^*(2) Mo_1$	0.14019	$\sigma^*Mo_1 - Mo_{13}$	0.46476	508.71	0.04	0.141	spd <sup>53.12%</sup>	s(26.73%) p(3.73%) d(69.54%)
	LPSi <sub>36</sub>	0.21354	$LP^*(3) Mo_{15}$	0.29182	446.11	0.15	0.363	spd	s(17.46%) p(76.72%) d(5.82%)
	$LP^*(2) Mo_1$	0.12019	$\sigma^*Mo_1 - S_2$	0.19660	358.71	0.01	0.141	spd <sup>69.56%</sup>	s(17.36%) p(38.91%) d(43.72%)
<b>MoS<sub>2</sub>_QD</b>	$LP^*(3) Mo_4$	0.34154	$LP^* Mo_{13}$	0.38483	700.05	0.01	0.143	Spd	s( 0.05%)p( 87.20%)d( 12.75%)
	$\pi Mo_1 - Mo_8$	0.65040	$\sigma^*Mo_1 - Mo_8$	0.36176	621.20	0.09	0.257	Spd <sup>50.00%</sup>	s( 14.17%)p( 24.84%)d( 60.98%)
<b>B@MoS<sub>2</sub>_NH<sub>3</sub></b>	$LP^*(2) Mo_{16}$	0.34380	$LP^*(2) Mo_5$	0.10959	4107.17	0.02	0.508	Spd	s( 0.91%)p( 92.76%)d( 6.34%)
	$\sigma^*Mo_8 - Mo_{14}$	0.59437	$\sigma^*Mo_8 - S_9$	0.27539	1353.59	0.02	0.221	Spd <sup>33.17%</sup>	s( 13.62%)p( 25.15%)d( 61.23%)
<b>N@MoS<sub>2</sub>_NH<sub>3</sub></b>	$\sigma^*Mo_8 - S_{11}$	0.28146	$\sigma^*Mo_8 - S_9$	0.24751	1892.76	0.02	0.312	Spd <sup>62.86%</sup>	s( 25.54%)p( 7.38%)d( 67.08%)
	$\sigma^*Mo_8 - S_{11}$	0.28146	$LP^* Mo_{14}$	0.35384	1091.40	0.02	0.198	Spd	s( 0.90%)p( 89.95%)d( 9.15%)
<b>P@MoS<sub>2</sub>_NH<sub>3</sub></b>	$LP Mo_{16}$	0.38509	$LP^* Mo_{15}$	0.36750	1012.07	0.02	0.201	Spd	s( 10.22%)p( 80.47%)d( 9.32%)
	$\sigma Mo_8 - S_9$	1.81052	$\pi Mo_1 - S_9$	1.86390	774.80	0.15	0.346	Spd <sup>41.87%</sup>	s( 12.41%)p( 10.15%)d( 77.44%)
<b>Si@MoS<sub>2</sub>_NH</b>	$\sigma^*Mo_{20} - S_{28}$	0.39827	$LPMo_{20}$	0.40970	645.69	0.04	0.216	Spd	s( 8.84%)p ( 65.52%)d ( 25.64%)
3	$\sigma^*Mo_{18} - S_{34}$	0.18666	$\sigma^*Mo_{18} - S_{24}$	0.32422	418.95	0.02	0.177	spd <sup>62.61%</sup>	s( 16.58%)p ( 8.07%)d ( 75.36%)
<b>S@MoS<sub>2</sub>_NH<sub>3</sub></b>	$LP^* Mo_{13}$	0.35435	$LP^*(2) Mo_1$	0.11457	477.23	0.01	0.132	Spd	s( 1.29%)p( 90.54%)d( 8.18%)
	$LP^* Mo_8$	0.17664	$\sigma^*Mo_8 - S_{11}$	0.25851	449.27	0.01	0.133	spd <sup>59.26%</sup>	s(8.61%) p(21.06%) d (70.33%)

