Supporting information：

Selective Sensing of NH_3 and NO_2 on WSe_2 Monolayer based on Defect Concentration Regulation

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Figure s1. The WSe_2 monolayer after optimization [11] (a) top view and (b) side view

Figure s2. Five optimized Se vacancy WSe_2 monolayers with (a) 2.000% (b) 3.125% (c) 5.556% (d) 8.333% (e) 12.500% V_{Se} concentration. The adsorption sites are also given, and the brown dotted circles represent the selenium vacancy.

Table s1 Defect formation energy (E_f/eV) of Se vacancy, W vacancy and Se on W antisite on WSe_2 monolayer [11].

Table s2. Initial configuration, adsorption distance (d/Å), adsorption energy (E_{ads}/eV), charge transfer number (Δq/e) and final configurations of NO_2 on perfect and five Se vacancy WSe_2 monolayers with different Se vacancy concentration. N up, NO_2; N down, O_2N; Single O downward, ONO, and parallel, p.

Table s3. Initial configuration, adsorption distance (d/Å), adsorption energy (E_{ads}/eV), charge transfer number (Δq/e) and final configurations of NH_3 on perfect and five Se vacancy WSe_2 monolayers with different Se vacancy concentration. NH_3, treble H downward; HNH_2, double H downward; H_2NH, single H downward; and H_3N, treble H upward.

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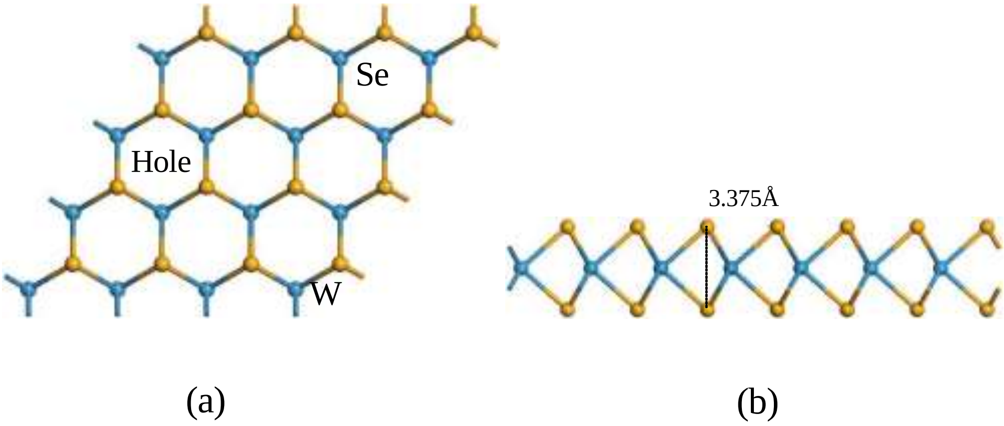

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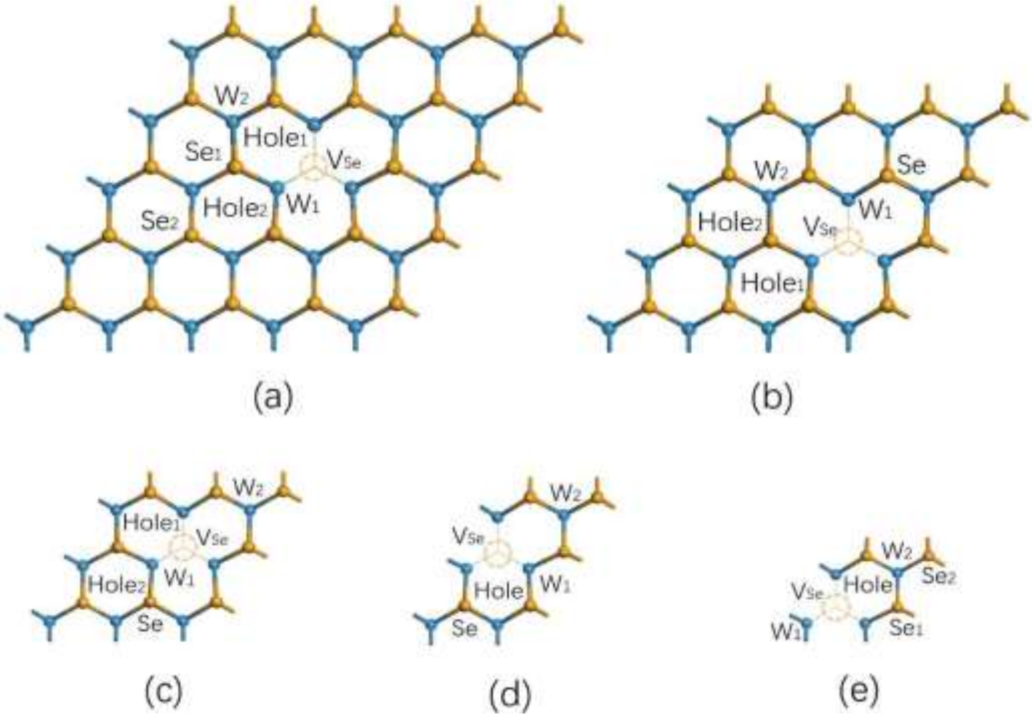

Figure s2. Five optimized Se vacancy WSe_2 monolayers with (a) 2.000% (b) 3.125% (c) 5.556% (d) 8.333% (e) 12.500% V_{Se} concentration. The adsorption sites are also given, and the brown dotted circles represent the selenium vacancy.

Table s1 Defect formation energy (E_f/eV) of Se vacancy, W vacancy and Se on W antisite on WSe_2 monolayer [11]

Defects	V_{Se}	V_W	Se_W	Ref
E_f/eV	2.70	4.95	4.72	This work
	2.70			30

The calculated formation energy order is E_f (V_W) ＞E_f (Se_W)＞E_f (V_{Se}) [11]. A single selenium vacancy has the lowest formation energy [11, 28-31].

Table s2. Initial configuration, adsorption distance (*d*/Å), adsorption energy (E_{ads}/eV), charge transfer number (Δq/e) and final configurations of NO_2 on perfect and five Se vacancy WSe_2 monolayers with different Se vacancy concentration. N up, NO_2; N down, O_2N; Single O downward, ONO; and parallel, p.

Vacancy concentration	**Initial configuration**	***d*/Å**	**E_{ads}/eV**	**Δq/e**	**Final configuration**
0[11]	**NO_2-hole**	**2.621**	**0.35**	**-0.205**	N upward
	NO_2-hole p	2.686	0.33	-0.200	
	NO_2-W	2.687	0.33	-0.200	
	NO_2-W p	2.695	0.33	-0.201	
	NO_2-Se	2.798	0.29	-0.192	
	NO_2-Se p	2.696	0.33	-0.200	
	ONO-hole	2.721	0.26	-0.193	
	ONO-W	2.640	0.35	-0.205	
	ONO-Se	2.735	0.29	-0.192	
	O_2N-hole	2.688	0.24	-0.185	N downward
	O_2N-W	2.776	0.22	-0.182	
	O_2N-Se	2.998	0.17	-0.175	
2.000%	NO_2-$hole_2$ p	2.631	0.40	-0.233	N upward
	NO_2-W_2	2.601	0.38	-0.231	
	ONO-W_2	2.607	0.38	-0.230	
	NO_2-W_2 p	2.603	0.37	-0.231	
	ONO-Se_1	2.637	0.37	-0.229	
	NO_2-W_1	2.108	0.35	-0.223	
	NO_2-Se_2 p	2.626	0.35	-0.233	
	ONO-$hole_2$	2.505	0.34	-0.226	
	NO_2-V_{Se}	2.141	0.34	-0.225	
	NO_2-$hole_2$	2.673	0.33	-0.223	
	ONO-Se_2	2.785	0.32	-0.221	
	NO_2-Se_2	2.815	0.32	-0.220	
	NO_2-Se_1 p	2.728	0.32	-0.217	
	NO_2-V_{Se} p	2.264	0.30	-0.222	
	NO_2-Se_1	2.759	0.30	-0.216	
	O_2N-W_1	1.615	0.41	-0.223	N downward
	O_2N-V_{Se}	1.668	0.40	-0.222	
	NO_2-W_1 p	1.599	0.38	-0.222	
	O_2N-W_2	2.703	0.25	-0.213	
	O_2N-$hole_2$	2.709	0.25	-0.214	
	O_2N-Se_1	2.979	0.19	-0.198	
	O_2N-$hole_1$	2.979	0.19	-0.198	

	O_2N-Se_2	2.998	0.19	-0.199	
	ONO-V_{Se}	**1.252**	**0.42**	**-0.221**	Single O downward
	NO_2-$hole_1$	1.860	0.37	-0.222	
	NO_2-$hole_1$ p	1.912	0.33	-0.222	
	ONO-W_1	2.959	0.12	-0.201	
	ONO-$hole_1$	2.959	0.12	-0.201	
3.125% [11]	NO_2-$hole_2$	2.587	0.35	-0.209	N upward
	NO_2-$hole_1$	2.641	0.35	-0.209	
	NO_2-W_2	2.608	0.35	-0.208	
	ONO-$hole_2$	2.607	0.35	-0.208	
	NO_2-$hole_2$ p	2.625	0.34	-0.206	
	NO_2-$hole_1$ p	2.645	0.33	-0.206	
	NO_2-W_2 p	2.652	0.33	-0.204	
	ONO-W_2	2.483	0.32	-0.200	
	NO_2-V_{Se}	2.074	0.31	-0.202	
	NO_2-Se	2.763	0.30	-0.198	
	NO_2-V_{Se} p	2.262	0.30	-0.196	
	ONO-Se	2.718	0.29	-0.198	
	NO_2-Se p	2.715	0.28	-0.195	
	ONO-$hole_1$	2.844	0.22	-0.191	
	NO_2-W_1 p	2.965	0.20	-0.188	
	O_2N-V_{Se}	1.582	0.40	-0.206	N downward
	ONO-W_1	1.590	0.38	-0.204	
	O_2N-$hole_2$	2.606	0.26	-0.186	
	O_2N-$hole_1$	2.649	0.25	-0.186	
	O_2N-W_2	2.740	0.22	-0.186	
	O_2N-Se	2.926	0.17	-0.178	
	NO_2-W_1	1.106	0.42	-0.208	Single O downward
	O_2N-W_1	1.097	0.42	-0.208	
	ONO-V_{Se}	1.567	0.40	-0.207	
5.556%	NO_2-$hole_2$	2.412	0.39	-0.141	N upward
	NO_2-Se	2.604	0.35	-0.197	
	ONO-W_2	2.617	0.33	-0.194	
	NO_2-$hole_1$	2.095	0.32	-0.187	
	NO_2-W_2	2.073	0.32	-0.186	
	ONO-$hole_2$	2.490	0.32	-0.191	
	NO_2-$hole_2$ p	2.417	0.32	-0.190	
	NO_2-V_{Se}	2.048	0.31	-0.195	
	NO_2-W_2 p	2.610	0.30	-0.188	
	ONO-Se	2.719	0.27	-0.184	
	NO_2-Se p	2.757	0.27	-0.184	
	O_2N-$hole_1$	1.524	0.40	-0.199	N downward
	O_2N-W_1	1.519	0.40	-0.199	

	O_2N-V_{Se}	2.318	0.27	-0.176	
	O_2N-$hole_2$	2.712	0.21	-0.171	
	O_2N-W_2	2.669	0.21	-0.167	
	O_2N-Se	2.955	0.15	-0.158	
	NO_2-W_1	**1.073**	**0.42**	**-0.205**	**Single O downward**
	ONO-$hole_1$	1.087	0.42	-0.204	
	NO_2-W_1 p	1.110	0.42	-0.203	
	NO_2-V_{Se} p	1.071	0.41	-0.207	
	ONO-V_{Se}	1.104	0.41	-0.204	
	NO_2-$hole_1$ p	1.102	0.41	-0.203	
	ONO-W_1	2.065	0.32	-0.186	
8.333%	NO_2-W_2 p	2.554	0.35	-0.185	N upward
	NO_2-V_{Se}	1.882	0.33	-0.190	
	NO_2-W_2	2.285	0.31	-0.171	
	ONO-W_2	2.409	0.31	-0.171	
	ONO-Se	2.719	0.28	-0.171	
	NO_2-Se	2.743	0.27	-0.170	
	NO_2-Se p	2.731	0.27	-0.169	
	NO_2-W_1 p	1.288	0.44	-0.197	N downward
	O_2N-V_{Se}	1.297	0.44	-0.196	
	O_2N-W_1	1.312	0.44	-0.196	
	O_2N-hole	1.642	0.44	-0.146	
	O_2N-W_2	2.659	0.21	-0.151	
	O_2N-Se	2.924	0.15	-0.144	
	NO_2-V_{Se} p	**-0.686**	**3.43**	**-0.644**	Single O downward
	NO_2-W_1	-0.688	3.43	-0.643	
	ONO-V_{Se}	-0.685	3.43	-0.642	
	ONO-W_1	-0.680	3.42	-0.644	
	ONO-hole	-0.679	3.42	-0.644	
	NO_2-hole	1.319	0.45	-0.151	
	NO_2-hole p	1.677	0.30	-0.170	
12.500%	NO_2-V_{Se}	1.979	0.42	-0.142	N upward
	NO_2-hole	2.158	0.39	-0.122	
	NO_2-Se_1 p	2.849	0.34	-0.116	
	NO_2-W_2 p	2.265	0.32	-0.162	
	NO_2-Se_1	2.903	0.32	-0.113	
	ONO-Se_2	2.702	0.29	-0.158	
	NO_2-Se_2	2.700	0.29	-0.157	
	NO_2-Se_2 p	2.702	0.28	-0.157	
	ONO-Se_1	2.677	0.26	-0.157	
	O_2N-hole	0.351	1.34	-0.228	N downward
	O_2N-V_{Se}	0.327	1.33	-0.229	
	O_2N-W_2	1.819	0.28	-0.090	

	O_2N-Se_1	3.118	0.23	-0.085	
	O_2N-Se_2	2.885	0.14	-0.126	
	ONO-V_{Se}	**-0.649**	**3.48**	**-0.638**	**Single O downward**
	NO_2-W_1 p	-0.650	3.48	-0.638	
	NO_2-W_1	-0.649	3.48	-0.637	
	NO_2-W_2	-0.647	3.48	-0.637	
	ONO-hole	-0.649	3.48	-0.637	
	ONO-W_1	-0.648	3.48	-0.637	
	O_2N-W_1	-0.650	3.47	-0.638	
	NO_2-V_{Se} p	-0.647	3.47	-0.637	
	NO_2-hole p	1.490	0.31	-0.175	
	ONO-W_2	2.628	0.12	-0.145	

Table s3. Initial configuration, adsorption distance (*d*/Å), adsorption energy (E_{ads}/eV), charge transfer number (Δq/e) and final configurations of NH_3 on perfect and five Se vacancy WSe_2 monolayers with different Se vacancy concentration. NH_3, treble H downward; HNH_2, double H downward; H_2NH, single H downward; and H_3N, treble H upward.

Vacancy concentration	**Initial configuration**	***d*/Å**	**E_{ads}/eV**	**Δq/e**	**Final configuration**
0	**NH_3-hole**	**2.714**	**0.37**	**0.040**	Treble H downward
	NH_3-W	2.745	0.36	0.048	
	NH_3-Se	3.094	0.29	0.028	
	HNH_2-W	2.608	0.33	0.015	Double H downward
	HNH_2-hole	2.640	0.33	0.011	
	HNH_2-Se	2.902	0.28	0.008	
	H_2NH-W	1.235	0.31	0.018	Single H downward
	H_2NH-hole	2.267	0.31	0.016	
	H_2NH-Se	2.704	0.27	-0.002	
	H_3N-hole	2.791	0.36	0.048	Treble H upward
	H_3N-W	2.813	0.35	0.045	
	H_3N-Se	3.389	0.26	0.018	
2.000%	NH_3-W_2	2.623	0.36	0.047	Treble H downward
	NH_3-$hole_2$	2.716	0.36	0.047	
	NH_3-W_1	2.434	0.34	0.037	
	NH_3-Se_1	3.028	0.29	0.029	
	NH_3-Se_2	3.097	0.29	0.026	
	HNH_2-W_2	2.606	0.56	0.013	Double H downward
	HNH_2-$hole_2$	2.648	0.38	0.013	
	HNH_2-Se_2	2.947	0.34	0.008	
	HNH_2-V_{Se}	1.246	0.29	0.076	
	HNH_2-Se_1	2.946	0.29	0.007	
	H_3N-$hole_1$	**0.772**	**0.56**	**0.094**	Single H downward
	NH_3-$hole_1$	0.767	0.56	0.093	
	H_2NH-W_1	0.782	0.56	0.093	
	NH_3-V_{Se}	0.770	0.56	0.092	
	H_2NH-V_{Se}	0.769	0.56	0.092	
	H_2NH-$hole_2$	2.272	0.56	0.017	
	HNH_2-W_1	0.770	0.36	0.092	
	H_2NH-W_2	2.216	0.31	0.018	
	HNH_2-$hole_1$	0.770	0.30	0.091	
	H_2NH-$hole_1$	2.322	0.28	0.007	
	H_2NH-Se_1	2.676	0.26	-0.001	

	H_2NH-Se_2	2.703	0.26	-0.001	
	H_3N-V_{Se}	1.806	0.38	0.046	Treble H upward
	H_3N-$hole_2$	2.726	0.37	0.056	
	H_3N-W_2	2.728	0.36	0.049	
	H_3N-W_1	2.665	0.32	0.039	
	H_3N-Se_1	3.330	0.26	0.020	
	H_3N-Se_2	3.388	0.26	0.019	
3.125%	NH_3-$hole_2$	2.613	0.37	0.054	Treble H downward
	NH_3-$hole_1$	2.622	0.36	0.057	
	H_2NH-$hole_1$	2.655	0.36	0.057	
	NH_3-W_2	2.727	0.36	0.041	
	NH_3-Se	3.028	0.29	0.029	
	HNH_2-$hole_2$	2.600	0.33	0.020	Double H downward
	HNH_2-W_2	2.666	0.33	0.010	
	HNH_2-W_1	2.646	0.30	0.003	
	HNH_2-Se	2.904	0.27	0.007	
	H_3N-V_{Se}	**0.736**	**0.57**	**0.099**	Single H downward
	NH_3-W_1	0.748	0.57	0.098	
	H_2NH-V_{Se}	0.753	0.57	0.096	
	H_2NH-W_1	0.755	0.57	0.096	
	HNH_2-V_{Se}	1.029	0.57	0.096	
	NH_3-V_{Se}	0.762	0.57	0.095	
	H_3N-W_1	2.174	0.34	0.030	
	H_2NH-$hole_2$	2.212	0.32	0.020	
	H_2NH-W_2	2.215	0.31	0.020	
	H_2NH-Se	2.658	0.26	0.004	
	H_3N-$hole_1$	2.688	0.37	0.057	Treble H upward
	HNH_2-$hole_1$	2.700	0.37	0.055	
	H_3N-$hole_2$	2.695	0.36	0.050	
	H_3N-W_2	2.871	0.34	0.042	
	H_3N-Se	3.327	0.26	0.020	
5.556%	NH_3-$hole_2$	2.666	0.36	0.052	Treble H downward
	NH_3-W_2	2.651	0.36	0.047	
	NH_3-Se	2.973	0.28	0.033	
	HNH_2-V_{Se}	1.263	0.51	0.078	Double H downward
	HNH_2-$hole_2$	2.666	0.33	0.014	
	HNH_2-W_1	2.565	0.32	0.017	
	HNH_2-W_2	2.614	0.32	0.017	
	HNH_2-$hole_1$	2.588	0.31	0.015	
	HNH_2-Se	2.966	0.28	0.007	
	H_3N-V_{Se}	**0.749**	**0.56**	**0.095**	Single H downward
	NH_3-V_{Se}	2.669	0.56	0.092	
	NH_3-W_1	0.760	0.56	0.092	

	H_2NH-V_{Se}	0.767	0.56	0.092	
	H_2NH-W_1	0.764	0.56	0.091	
	NH_3-$hole_1$	0.769	0.56	0.090	
	H_2NH-Se	2.716	0.36	0.050	
	H_2NH-W_2	2.252	0.31	0.014	
	H_2NH-$hole_1$	2.286	0.29	0.010	
	H_3N-$hole_2$	2.697	0.36	0.054	Treble H upward
	H_3N-W_2	2.820	0.34	0.042	
	H_3N-$hole_1$	2.825	0.30	0.034	
	H_3N-W_1	2.822	0.30	0.028	
	H_3N-Se	3.387	0.25	0.017	
	H_2NH-$hole_2$	2.728	0.25	-0.004	
8.333%	NH_3-W_2	2.626	0.35	0.056	Treble H downward
	NH_3-Se	3.112	0.27	0.031	
	HNH_2-W_2	2.589	0.33	0.011	Double H downward
	HNH_2-Se	2.893	0.27	0.009	
	HNH_2-W_1	**0.754**	**0.56**	**0.093**	Single H downward
	H_3N-V_{Se}	0.766	0.56	0.091	
	HNH_2-hole	0.764	0.56	0.091	
	NH_3-hole	0.764	0.56	0.090	
	NH_3-VSe	0.770	0.56	0.089	
	H_2NH-V_{Se}	0.784	0.56	0.088	
	HNH_2-V_{Se}	0.771	0.56	0.088	
	H_2NH-hole	0.782	0.56	0.087	
	NH_3-W_1	0.762	0.56	0.085	
	H_2NH-W_1	0.767	0.50	0.089	
	H_2NH-W_2	2.250	0.31	0.014	
	H_2NH-Se	2.731	0.26	-0.003	
	H_3N-W_2	2.794	0.32	0.043	Treble H upward
	H_3N-hole	2.754	0.30	0.034	
	H_3N-W_1	2.966	0.28	0.019	
	H_3N-Se	3.430	0.24	0.014	
12.500%	NH_3-W_2	2.722	0.34	0.060	Treble H downward
	NH_3-Se_1	3.052	0.26	0.039	
	NH_3-Se_2	3.081	0.26	0.039	
	HNH_2-W_2	2.622	0.32	0.016	Double H downward
	HNH_2-Se_1	3.020	0.27	0.006	
	HNH_2-Se_2	3.019	0.27	0.005	
	NH_3-W_1	**0.752**	**0.57**	**0.091**	Single H downward
	HNH_2-V_{Se}	0.769	0.57	0.089	
	HNH_2-W_1	0.775	0.57	0.089	
	NH_3-hole	0.768	0.57	0.088	
	H_3N-hole	0.773	0.57	0.087	

	H_2NH-V_{Se}	0.773	0.57	0.086	
	H_3N-V_{Se}	0.771	0.56	0.090	
	HNH_2-hole	0.771	0.56	0.090	
	H_2NH-hole	0.774	0.56	0.089	
	H_2NH-W_1	0.778	0.56	0.087	
	NH_3-V_{Se}	0.903	0.55	0.080	
	H_2NH-W_2	2.265	0.31	0.016	
	H_2NH-Se_1	2.755	0.26	0.000	
	H_3N-Se_1	2.779	0.26	-0.001	
	H_2NH-Se_2	2.753	0.26	-0.001	
	H_3N-W_2	2.879	0.30	0.036	Treble H upward
	H_3N-W_1	2.881	0.27	0.021	
	H_3N-Se_2	3.445	0.22	0.013	