

Supporting Information

Potential Applications of Defective NiCl₂ Monolayer as Toxic Gas Sensors: A Computational Study

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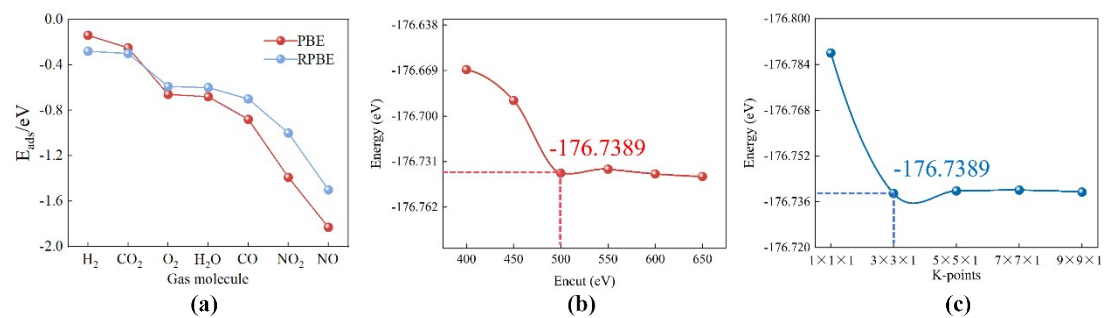


Fig. S1. Adsorption energies calculated by PBE and RPBE functionals (a), computed total energies of VCl-NiCl₂ by considering different cutoff energy (b) and K-points (c) and the adopted energies in the present work.

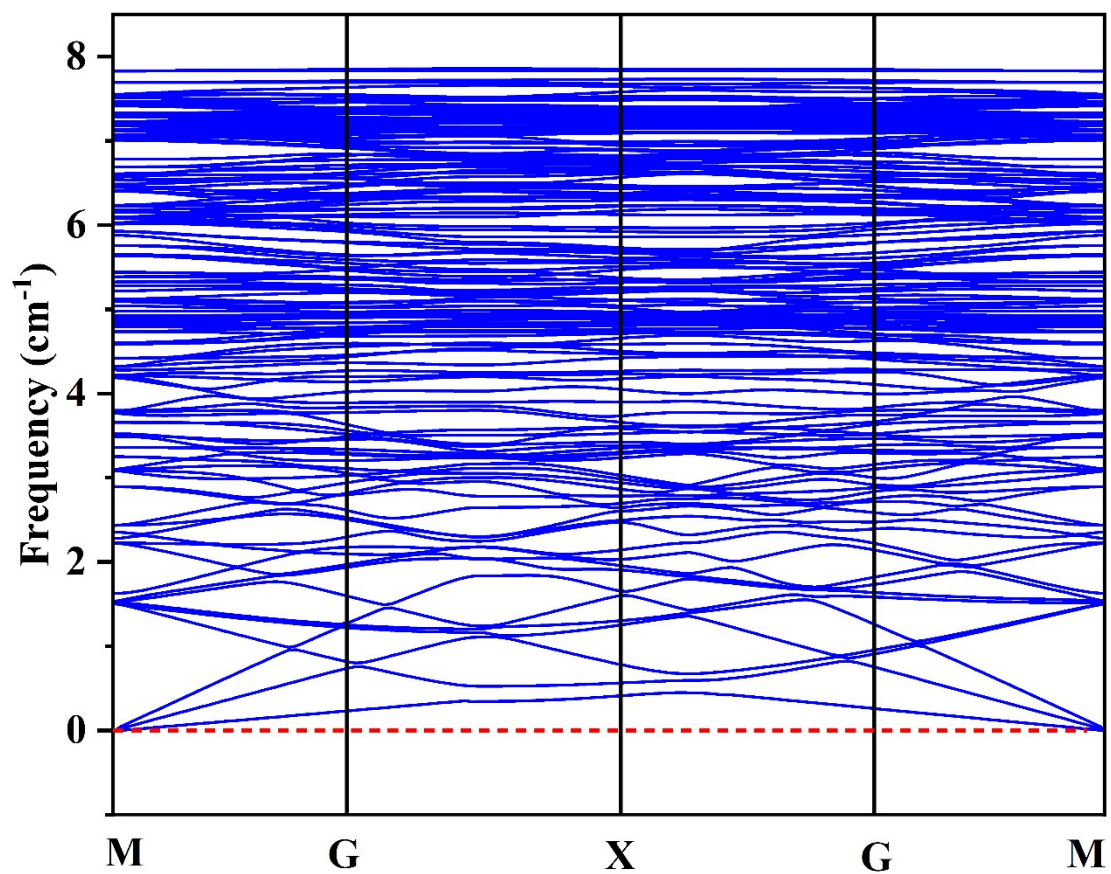


Fig. S2. The computed phonon dispersions of V_{Cl} - $NiCl_2$ monolayer.

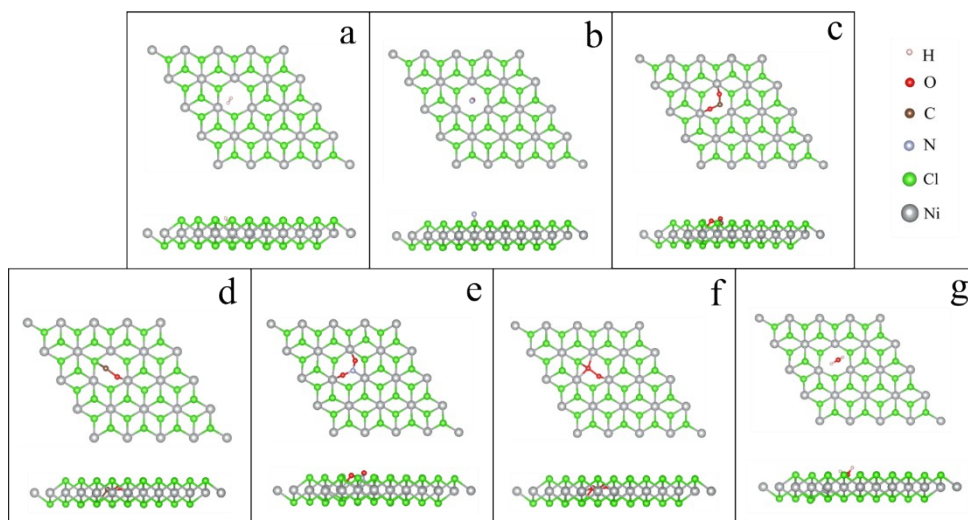


Fig. S3. Optimized suitable structures for (a) H_2 , (b) NO , (c) CO_2 , (d) CO , (e) NO_2 , (f) O_2 , and (g) H_2O adsorbed on V_{Cl} - $NiCl_2$ monolayer.

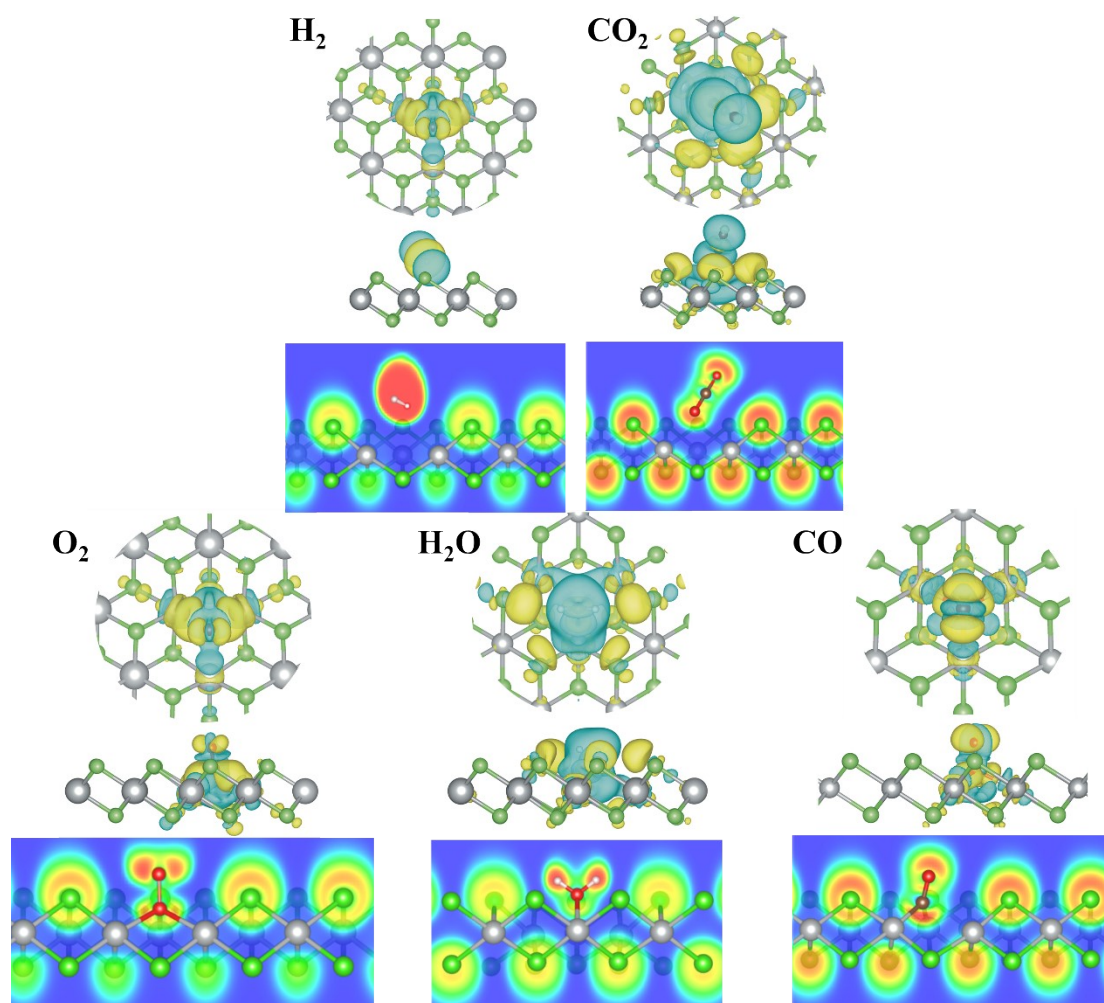


Fig. S4 Difference charge density and ELF maps of small molecules adsorbed on V_{Cl} - $NiCl_2$, the iso-surface value is $0.02 e \text{ \AA}^{-3}$. The charge accumulation and disruption regions are shown in yellow and cyan, respectively.

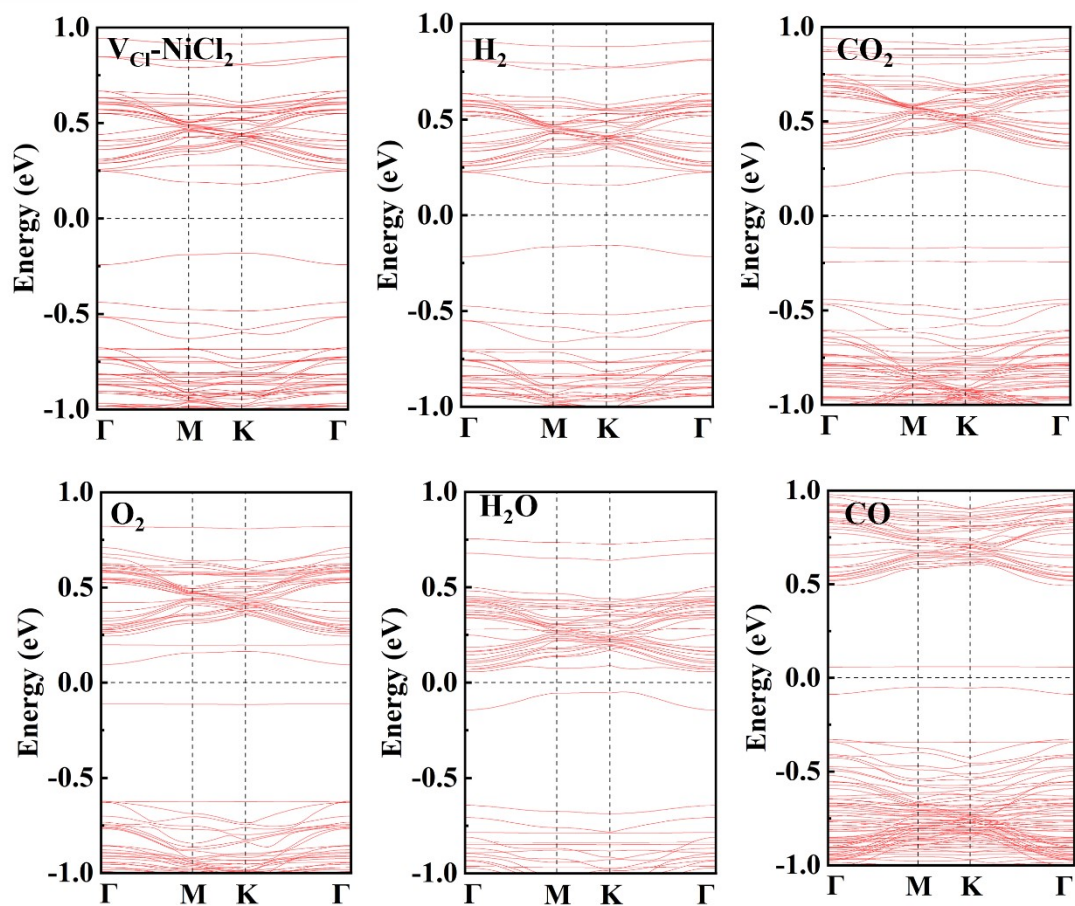


Fig. S5 Computed band structures of $V_{Cl}-NiCl_2$ monolayer, H_2 , CO_2 , O_2 , H_2O and CO adsorbed on $V_{Cl}-NiCl_2$ monolayer.

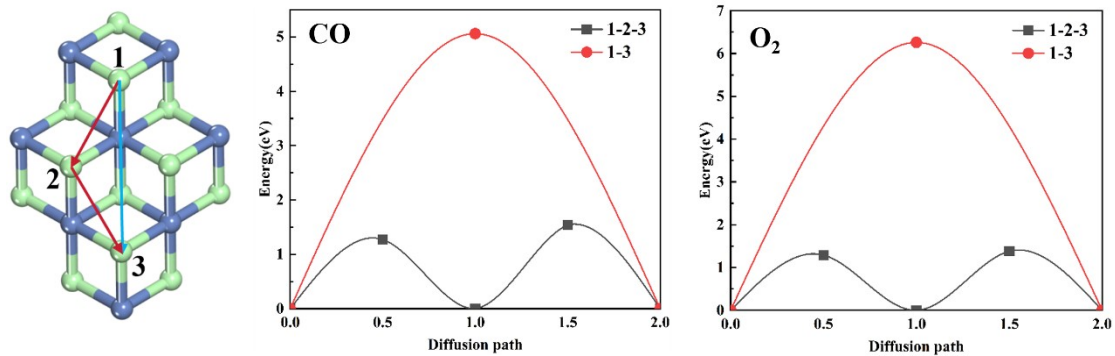


Fig. S6 (a) The selected adsorption sites and diffusion paths, and diffusion barriers of CO and O₂.

Cartesian coordination information of $V_{Cl-NiCl_2}$.

defective $NiCl_2$

1.0

13.9425001144	0.0000000000	0.0000000000
-6.9715024842	12.0744135491	0.0000000000
0.0029667614	-0.0017128192	19.9999997066

Cl	Ni
31	16

Cartesian

1.742889846	1.008398204	6.302599814
0.006710366	2.026615239	3.696399873
5.227190164	1.005138183	6.302599814
3.480414655	2.026253072	3.696199899
8.714349342	1.002240171	6.303599980
6.970152301	2.010436120	3.689199930
12.201716360	1.005017468	6.301399973
10.459401772	2.010919101	3.688400036
0.011585197	4.071194221	6.301599649
-1.798844571	4.997771316	3.638199812
3.474832820	4.070831890	6.301199701
1.743332162	5.093269998	3.751800005
6.969452103	4.025794202	6.302800086
5.285897302	4.997771316	3.638199812
10.460374893	4.026518503	6.303599980
8.715131822	5.032903349	3.689199930
-1.695875328	7.028459789	6.301399973
-3.469908222	8.047038620	3.696599846
0.054624980	8.018055495	3.752199952
5.183145488	7.029304724	6.301199701
3.431568965	8.018175683	3.752199952
8.714223175	7.045001068	6.302599814
6.956432944	8.047279733	3.696399873
-3.481693723	10.059620279	6.302199867
-5.227634366	11.067695611	3.684399968
0.036417723	10.028709613	6.301399973
-1.732735598	11.055741216	3.696599846
3.451075451	10.028709613	6.301399973
1.743467677	11.133143224	3.638400084
6.969116279	10.060706978	6.302599814
5.219762041	11.055378526	3.696199899
13.941707052	0.000538553	4.990599976
3.487689813	0.000417809	4.990599976
0.006343673	12.073261489	4.989799784
3.480117237	12.073503322	4.989599810
-1.744784657	3.023730289	4.989599810
1.743284057	3.030610401	5.016400144
5.231345181	3.023730289	4.989599810
8.714948814	3.018055413	4.988799916

-3.481455676	6.032070504	4.989799784
-0.058094393	6.002494435	4.914199936
3.544786527	6.002736251	4.914199936
6.968168880	6.032070521	4.989599810
8.714544188	9.053813116	4.990599976
-1.730964187	9.048860151	5.016400144
1.743768750	9.123247542	4.914199936
5.218186490	9.049222875	5.016400144