

Defective Cr₂CT_x-Based Sensors with Highly Sensitivity for NO₂ Detection at Room Temperature

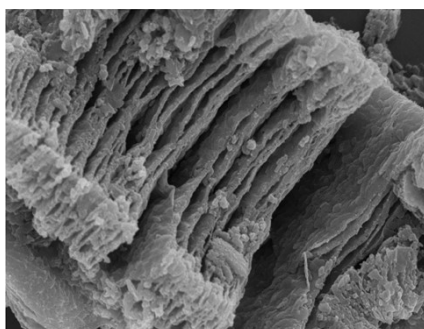


Fig. S1. The SEM image of multilayer Cr₂CT_x particle.

Table S1. Comparison of the response, response/recovery time of Cr₂CT_x to different concentrations of NO₂.

Concentration	Response (%)	Response/recovery time (s)
100 ppb	2.32	66/127
1 ppm	14.01	80/239
5 ppm	37.98	84/247
10 ppm	62.35	88/245
30 ppm	76.91	102/252
50 ppm	85.40	112/257

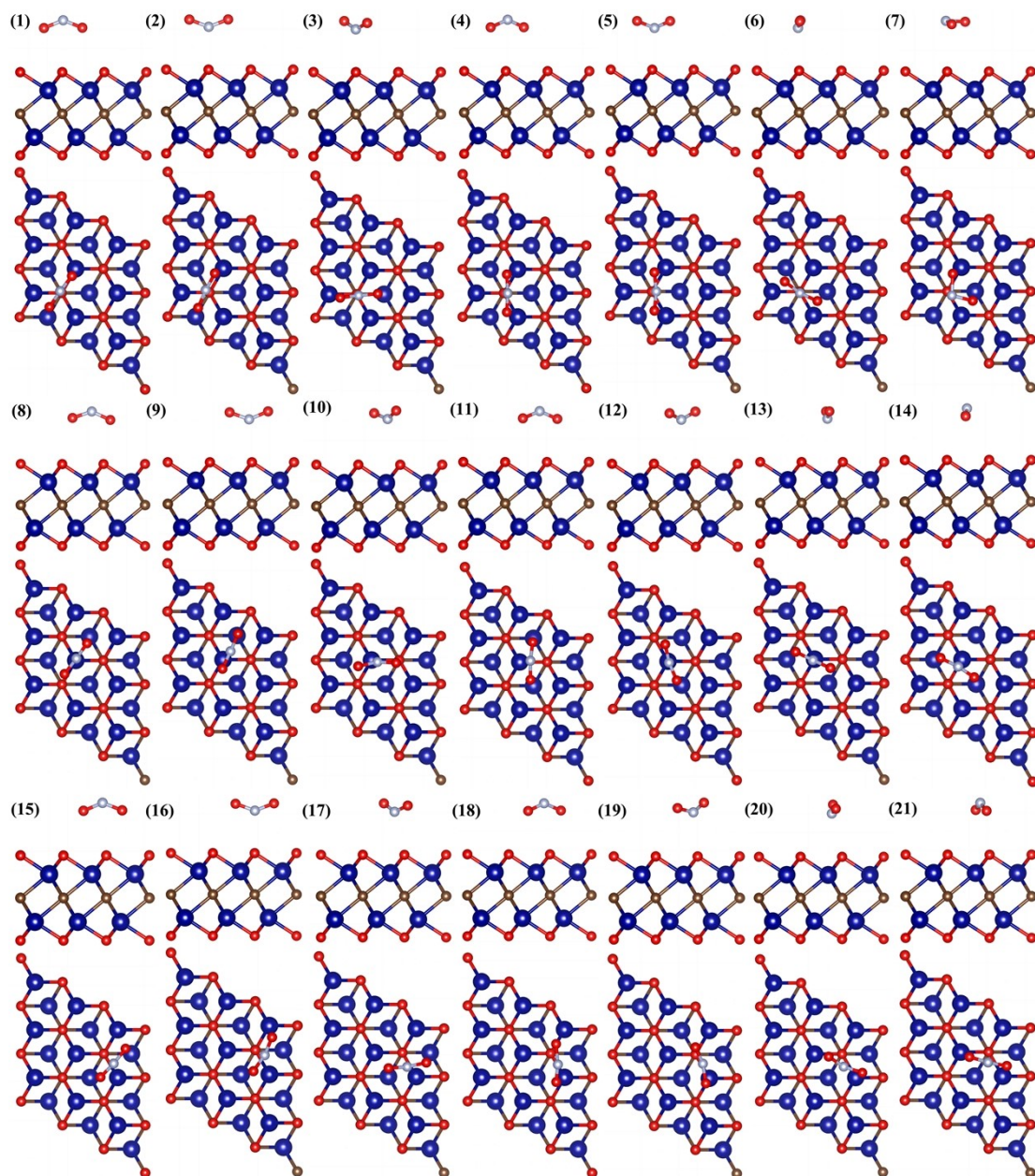


Fig. S2. Different adsorption configurations of NO_2 molecules on Cr_2CO_2 surfaces.

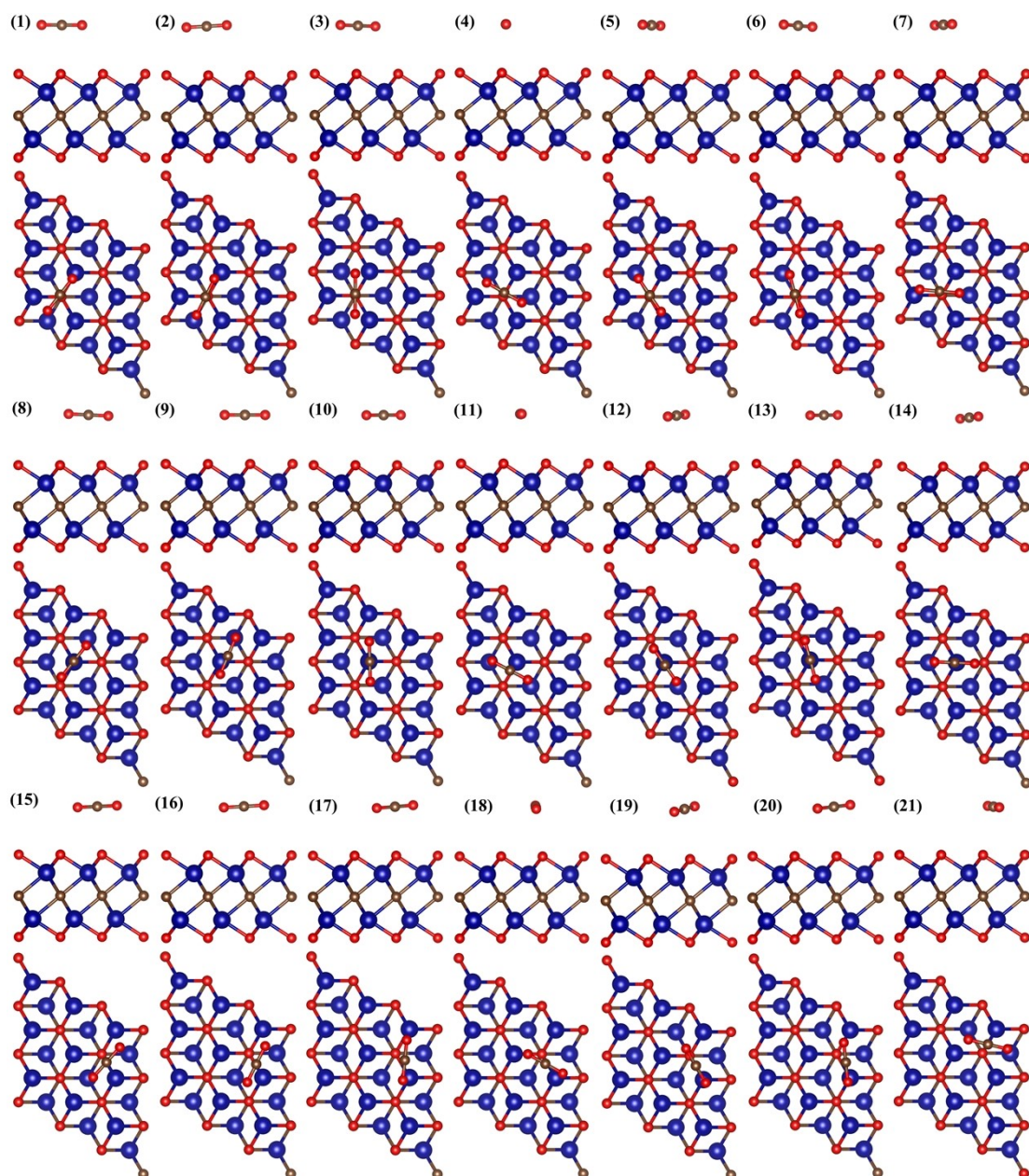


Fig. S3. Different adsorption configurations of CO₂ molecules on Cr₂CO₂ surfaces.

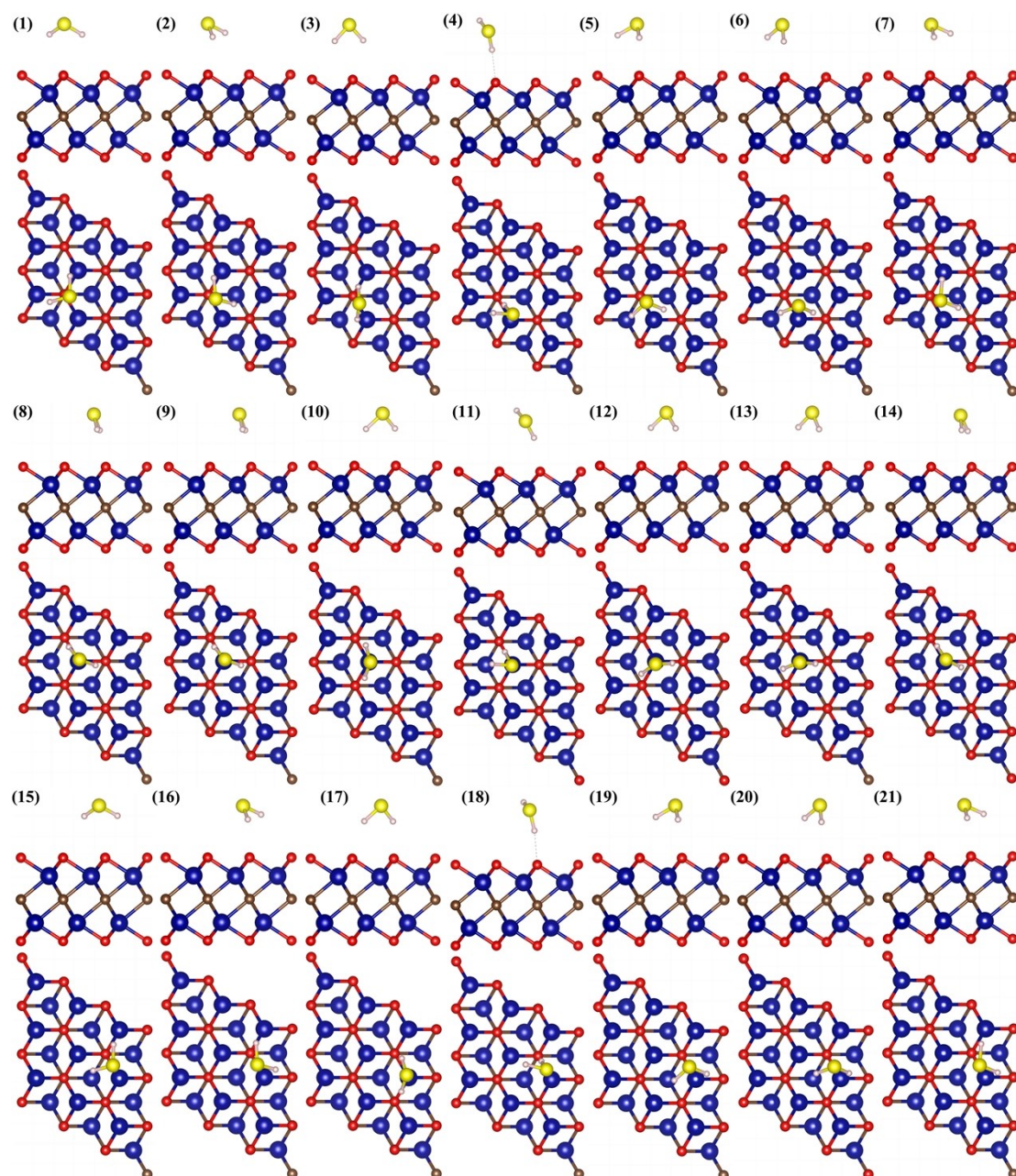


Fig. S4. Different adsorption configurations of H_2S molecules on Cr_2CO_2 surfaces.

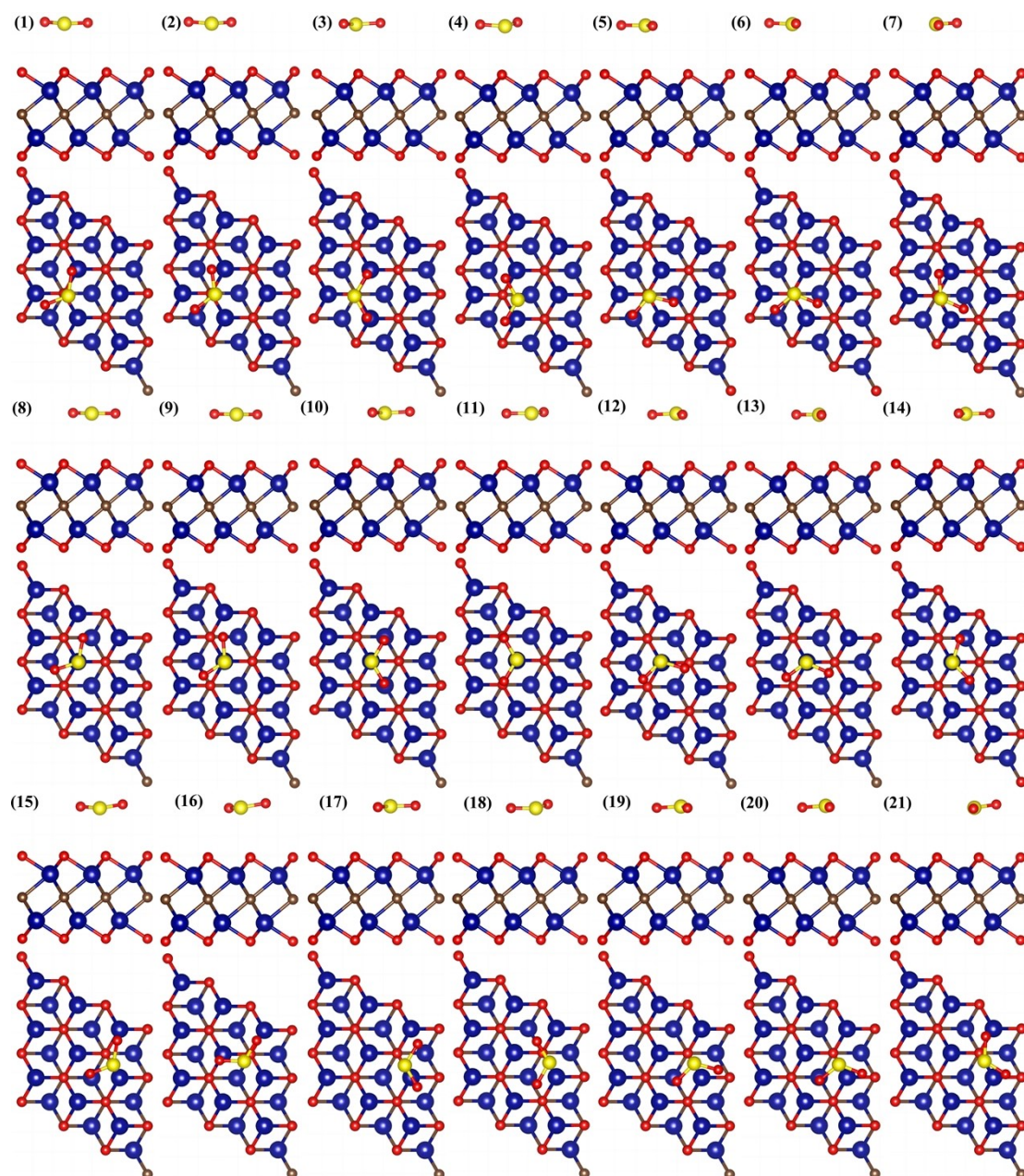


Fig. S5. Different adsorption configurations of SO_2 molecules on Cr_2CO_2 surfaces.

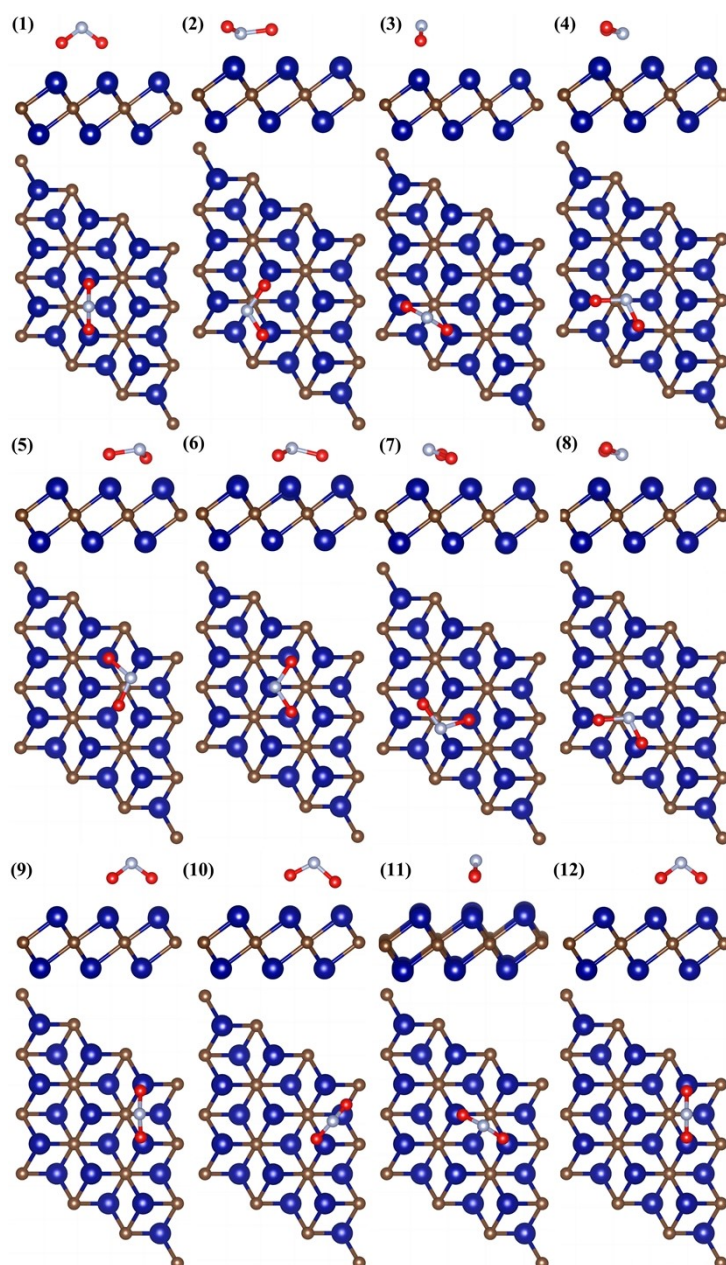


Fig. S6. Different adsorption configurations of NO_2 molecules on Cr_2C surfaces.

Table S2

The corresponding calculated adsorption energies (eV/molecule) for different models given in Figure S1-S4.

Model No.	NO_2	CO_2	H_2S	SO_2
1	-0.531	-0.183	-0.271	-0.256
2	-0.517	-0.184	-0.297	-0.256
3	-0.514	-0.181	-0.283	-0.258
4	-0.530	-0.182	-0.278	-0.250
5	-0.517	-0.183	-0.292	-0.258
6	-0.515	-0.181	-0.305	-0.258
7	-0.513	-0.181	-0.290	-0.257
8	-0.507	-0.167	-0.292	-0.240

9	-0.522	-0.180	-0.319	-0.229
10	-0.277	-0.167	-0.318	-0.248
11	-0.534	-0.177	-0.285	-0.217
12	-0.289	-0.170	-0.316	-0.222
13	-0.290	-0.165	-0.313	-0.228
14	-0.528	-0.169	-0.316	-0.244
15	-0.340	-0.183	-0.275	-0.250
16	-0.520	-0.178	-0.300	-0.248
17	-0.518	-0.181	-0.317	-0.248
18	-0.305	-0.177	-0.272	-0.244
19	-0.508	-0.173	-0.304	-0.247
20	-0.327	-0.177	-0.298	-0.249
21	-0.530	-0.182	-0.292	-0.249

Table S3

The corresponding calculated adsorption energies (eV/molecule) for different models given in Figure S5.

Model No.	Adsorption energy (E_{ads}) of the NO ₂ gas
1	-2.927
2	-1.990
3	-2.927
4	-3.197
5	-3.491
6	-3.677
7	-3.492
8	-3.200
9	-2.927
10	-2.868
11	-2.926
12	-2.927