

**Table S1.** The bond length changes of SF<sub>6</sub> molecules after adsorption.

Covalent bond	Bond length before adsorption (Å)	Bond length after adsorption (Å)	Variable quantity (Å)
S(1) - F(1)	1.581	1.57736	-0.00364
S(1) - F(2)	1.581	1.57412	-0.00688
S(1) - F(3)	1.581	1.59365	0.01265
S(1) - F(4)	1.581	1.59342	0.01242
S(1) - F(5)	1.581	1.57721	0.00379
S(1) - F(6)	1.581	1.57991	-0.00109

**Table S2.** The bond angle changes of SF<sub>6</sub> molecules after adsorption.

Bond angle	Before adsorption (°)	After adsorption (°)	Variable quantity (°)
F(1) - S(1) - F(2)	90.00	90.2946	0.2946
F(1) - S(1) - F(3)	90.00	90.1272	0.1272
F(1) - S(1) - F(4)	180.00	179.3257	-0.6743
F(1) - S(1) - F(5)	90.00	90.5797	0.5797
F(1) - S(1) - F(6)	90.00	89.8415	-0.1585
F(2) - S(1) - F(3)	180.00	178.8050	-1.1950
F(2) - S(1) - F(4)	90.00	90.2133	0.2133
F(2) - S(1) - F(5)	90.00	90.2800	0.2800
F(2) - S(1) - F(6)	90.00	90.2171	0.2171
F(3) - S(1) - F(4)	90.00	89.3615	-0.6385
F(3) - S(1) - F(5)	90.00	88.3615	-0.6385
F(3) - S(1) - F(6)	90.00	89.3350	-0.6650
F(4) - S(1) - F(5)	90.00	89.8613	-0.1387
F(4) - S(1) - F(6)	90.00	89.7130	-0.2870
F(5) - S(1) - F(6)	180.00	179.3468	-0.6532

**Table S3.** The bond length changes of CF<sub>4</sub> molecules after adsorption.

Covalent bond	Bond length before adsorption (Å)	Bond length after adsorption (Å)	Variable quantity (Å)
C(1) - F(1)	1.316	1.31369	-0.00231
C(1) - F(2)	1.316	1.32503	0.00903
C(1) - F(3)	1.316	1.32504	0.00904
C(1) - F(4)	1.316	1.30540	-0.01060

**Table S4.** The bond angle changes of CF<sub>4</sub> molecules after adsorption.

Bond angle	Before adsorption (°)	After adsorption (°)	Variable quantity (°)
F(1) - C(1) - F(2)	109.47	108.7871	-0.6829
F(1) - C(1) - F(3)	109.47	108.8117	-0.6583
F(1) - C(1) - F(4)	109.47	109.9602	0.4902
F(2) - C(1) - F(3)	109.47	108.9077	-0.5623
F(2) - C(1) - F(4)	109.47	110.1150	0.6450
F(3) - C(1) - F(4)	109.47	110.1830	0.7130

**Table S5.** The bond length changes of CS<sub>2</sub> molecules after adsorption.

Covalent bond	Bond length before adsorption (Å)	Bond length after adsorption (Å)	Variable quantity (Å)
C(1) - S(1)	1.5562	1.55659	0.00039
C(1) - S(2)	1.5562	1.55650	0.00030

**Table S6.** The bond angle changes of CS<sub>2</sub> molecules after adsorption.

Bond angle	Before adsorption (°)	After adsorption (°)	Variable quantity (°)
S(1) - C(1) - S(2)	180.00	179.9421	-0.05790

**Table S7.** The bond length changes of SO<sub>2</sub> molecules after adsorption.

Covalent bond	Bond length before adsorption (Å)	Bond length after adsorption (Å)	Variable quantity (Å)
S(1) - O(1)	1.454	1.4605	0.00650
S(1) - O(2)	1.454	1.4605	0.00650

**Table S8.** The bond angle changes of SO<sub>2</sub> molecules after adsorption.

Bond angle	Before adsorption (°)	After adsorption (°)	Variable quantity (°)
O(1) - S(1) - O(2)	118.59	117.5156	-1.0744

**Table S9.** The bond length changes of SO<sub>2</sub>F<sub>2</sub> molecules after adsorption.

Covalent bond	Bond length before adsorption (Å)	Bond length after adsorption (Å)	Variable quantity (Å)
S(1) - F(1)	1.575	1.55352	-0.02148
S(1) - F(2)	1.575	1.55660	-0.01840
S(1) - O(1)	1.424	1.42192	-0.00208
S(1) - O(2)	1.424	1.42251	-0.00149

**Table S10.** The bond angle changes of SO<sub>2</sub>F<sub>2</sub> molecules after adsorption.

Bond angle	Before adsorption (°)	After adsorption (°)	Variable quantity (°)
F(1) - S(1) - F(2)	94.8349	95.5080	0.6731
F(1) - S(1) - O(1)	107.9328	108.1127	0.1799
F(1) - S(1) - O(2)	107.9394	108.1244	0.1850
F(2) - S(1) - O(1)	107.9328	105.7185	-2.2143
F(2) - S(1) - O(2)	107.9394	105.6996	-2.2398
O(1) - S(1) - O(2)	125.8551	128.6210	2.7659

**Table S11.** The bond length changes of SOF<sub>2</sub> molecules after adsorption.

Covalent bond	Bond length before adsorption (Å)	Bond length after adsorption (Å)	Variable quantity (Å)
S(1) - F(1)	1.616	1.6250	0.0090
S(1) - F(2)	1.616	1.5900	-0.0260
S(1) - O(1)	1.437	1.4470	0.0100

**Table S12.** The bond angle changes of SOF<sub>2</sub> molecules after adsorption.

<b>Bond angle</b>	<b>Before adsorption (°)</b>	<b>After adsorption (°)</b>	<b>Variable quantity (°)</b>
F(1) - S(1) - F(2)	92.64	94.27	1.6300
F(1) - S(1) - O(1)	106.71	108.17	1.4600
F(2) - S(1) - O(1)	106.71	106.13	-0.5800