Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supporting information

Degradation and adsorption of SF_6 decomposition components using AlN nanocones: a combination of DFT and ab initio molecular dynamics study

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The molecular electrostatic potential surface

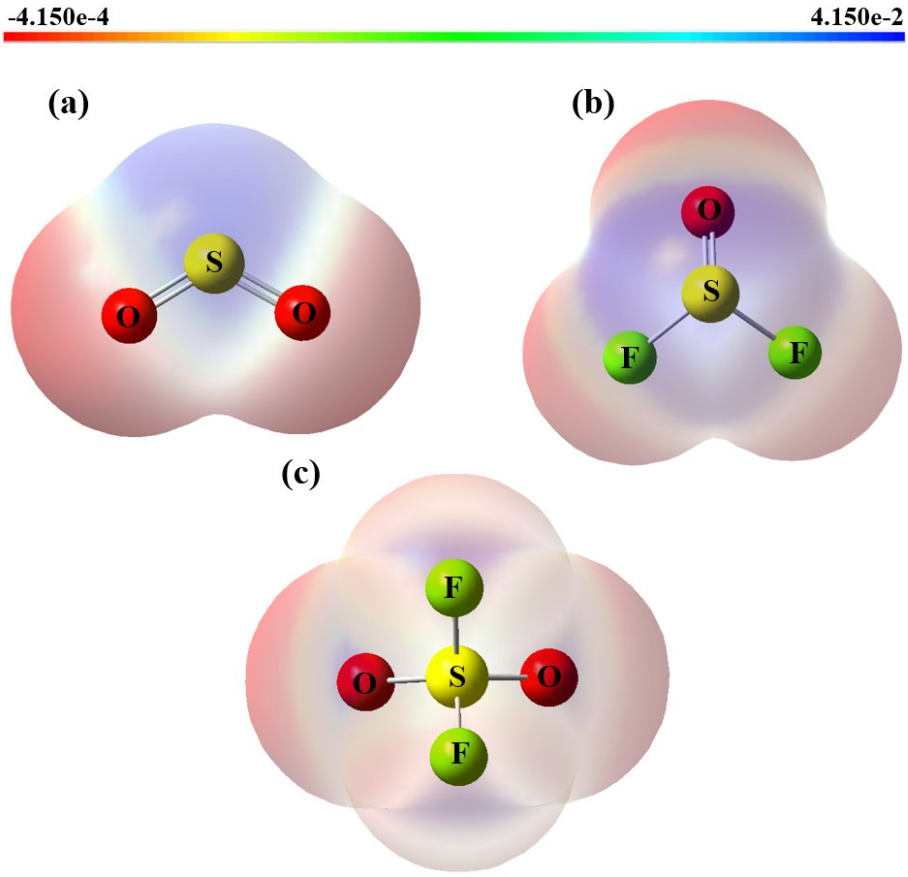

Figure S1. Molecular electrostatic potential surface of (a) SO_2, (b) SOF_2, and (c) SO_2F_2 gas molecules. Where the red color indicates areas of high negative potential, while blue color represents regions of high positive potential. The intensity of the red or blue color reflects the magnitude of the potential.

The HOMO-LUMO profiles

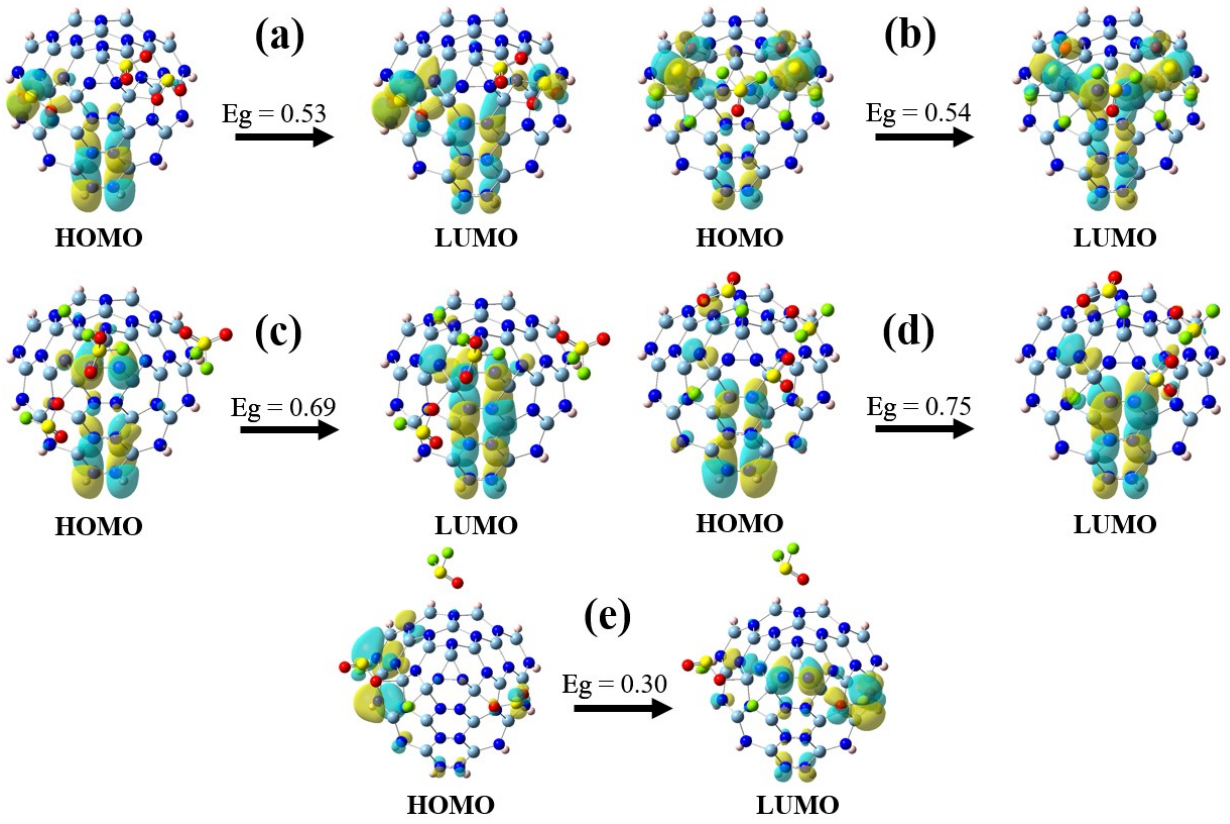

Figure S2. HOMO-LUMO profiles related to dominant structure of (a) AlNNC@SO_2, (b) AlNNC@SOF_2, (c) AlNNC@SO_2F_2, (d) AlNNC@Top, (e) AlNNC@Side systems. Where Eg is energy gap between HOMO-LUMO in eV.

The angle distributions of AlNNC@SO_2, AlNNC@SOF_2, AlNNC@SO_2F_2, and AlNNC@Side

In the case of AlNNC@SO_2, O1-Al1 creates a strong about (97˚, 1.85 Å) while O2-Al3 creates a weaker bond varied about 1.9-2.0 Å. Where diagonal angular changes of θ2 and θ3 along with variable S2-N2 bond length around 1.85-1.95 Å, indicate the tendency of S3 to make a bond with N. In addition, O3-S3-O4 can make a stronger bond from its O3 side (105˚, 1.88 Å) with Al2, **Figure S3**.

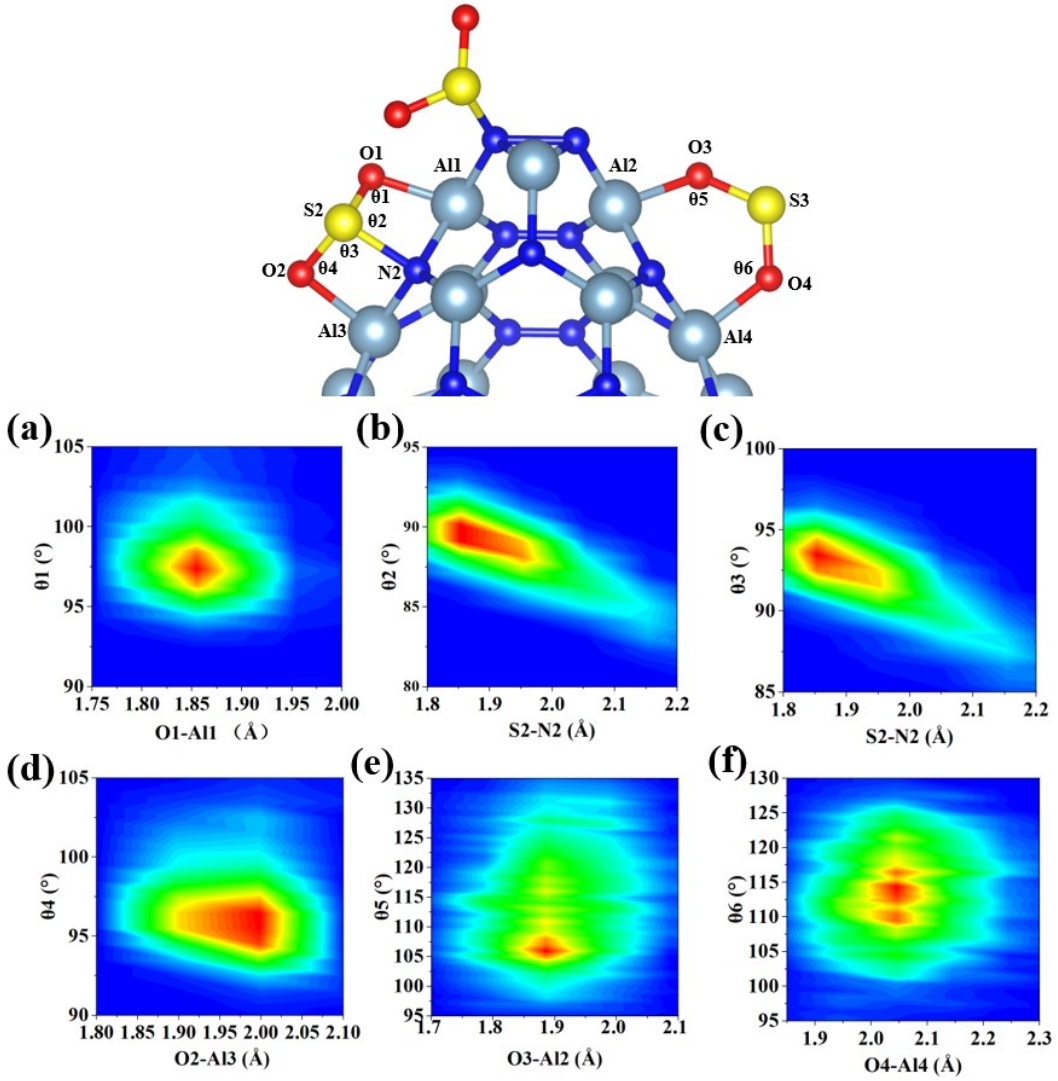

Figure S3. Angular analysis related to dominant structure of AlNNC@SO_2.

The result of angular distribution for AlNNC@SOF_2 showed that each of S1-O1 and S2-O2 forms a strong quadrilateral cluster with AlNNC surface, in which θ1, θ2, θ3, and θ4 make angles about 93˚. where S-N bonds (S1-N1 and S2-N2) make smaller bonds than O-Al bonds (O1-Al3 and O2-Al4), **Figure S4**.

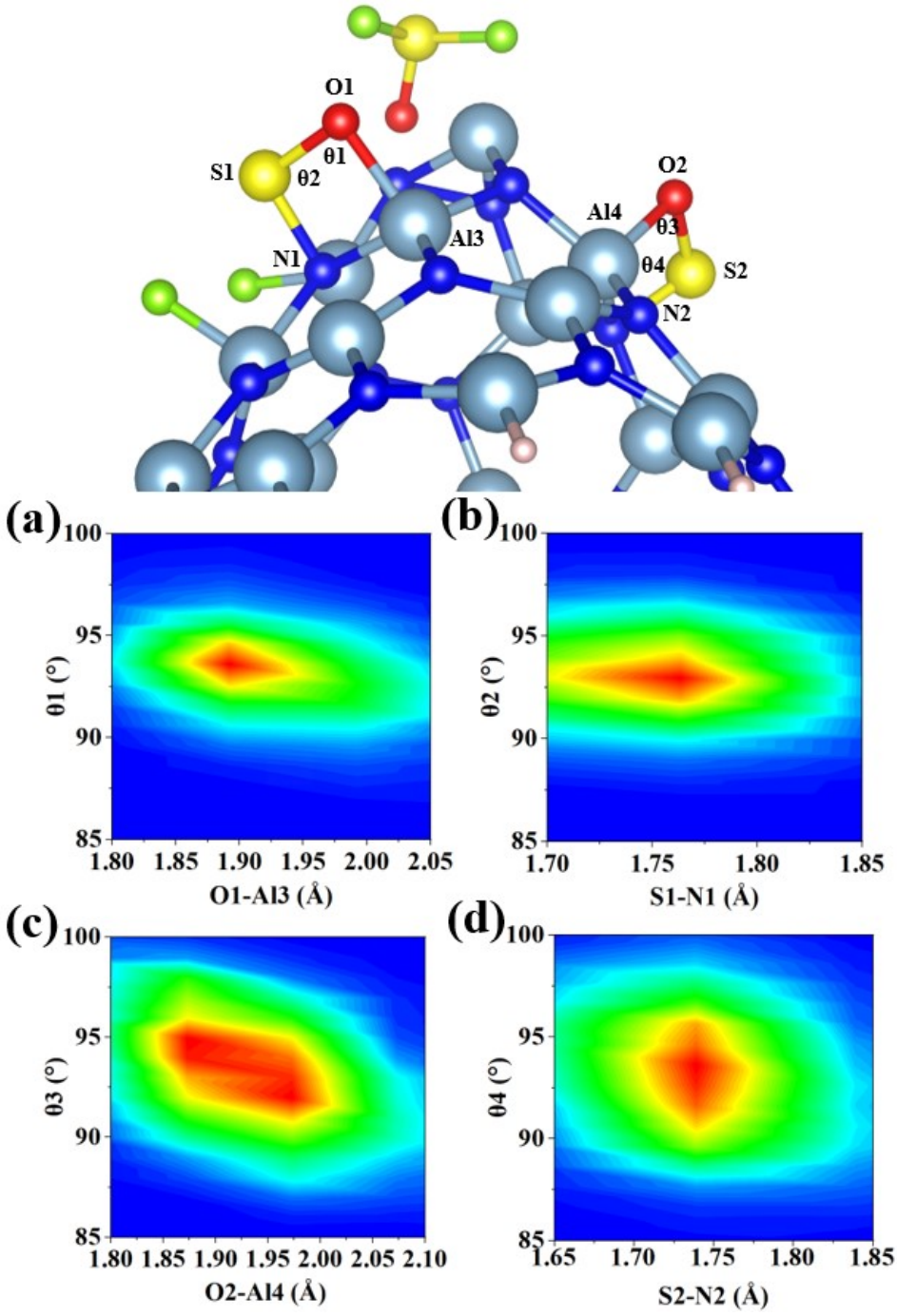

Figure S4. Angular analysis related to dominant structure of AlNNC@SOF_2.

In the case of AlNNC@SO_2F_2, O1Al1 and O2Al3 almost make the same bond length with the AlNNC surface but with different angles; however, θ2 can be more stable than θ1, which can be affected by the electronegativity of fluorine atom, **Figure S5**.

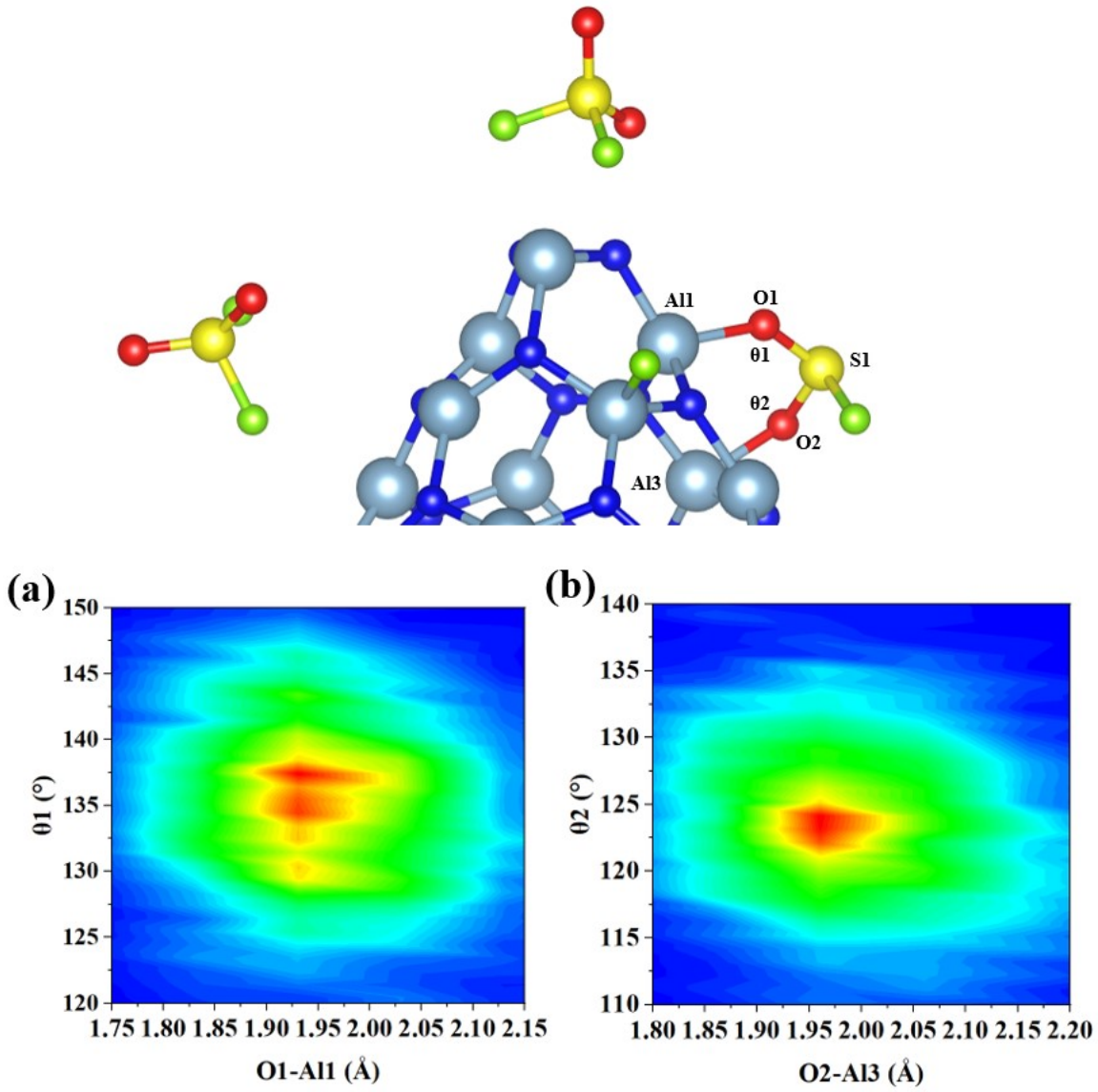

Figure S5. Angular analysis related to dominant structure of AlNNC@SO_2F_2.

In the case of AlNNC@Side, S1-O1 makes the strongest bond with AlNNC surface about <1.93 Å bond length, while S2-O3 makes a weak but with stable angular to AlNNC about (134˚, 2.05 Å), **Figure S6**.

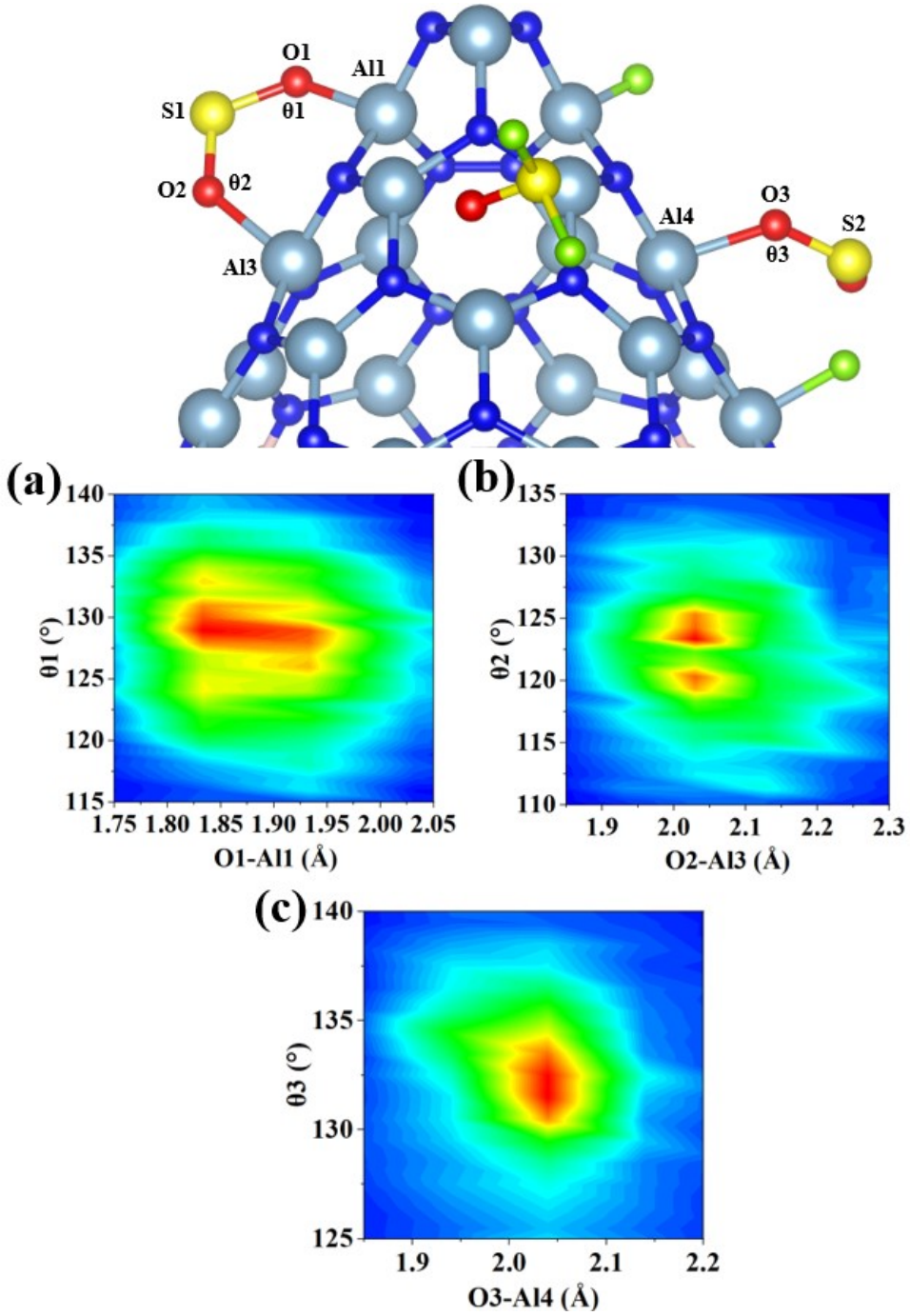

Figure S6. Angular analysis related to dominant structure of AlNNC@Side.

The atomic partial charges in the most stable structures

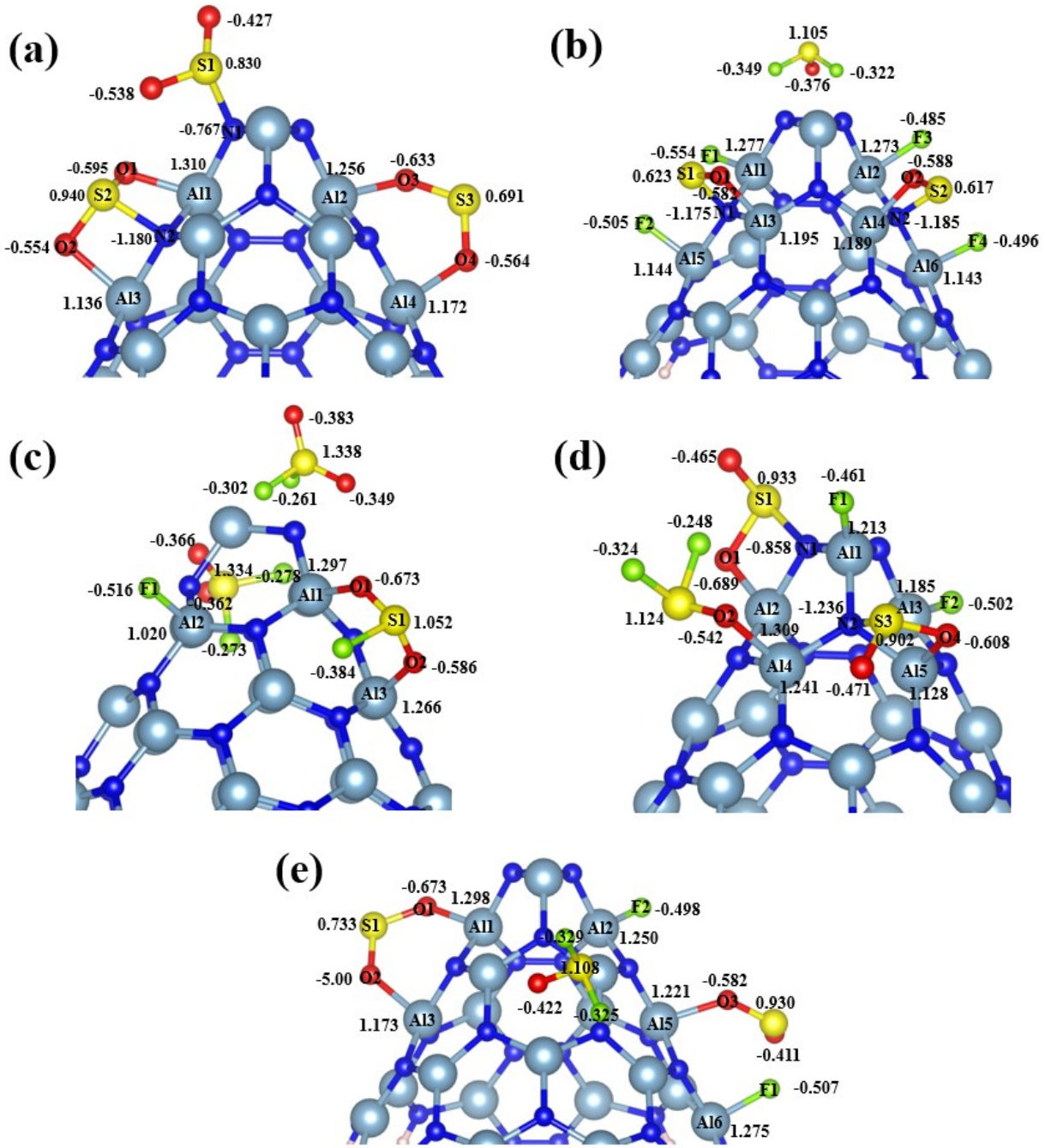

Figure S7. The atomic partial charges placed on the atoms in the most stable structures of (a) AlNNC@SO_2, (b) AlNNC@SOF_2, (c) AlNNC@SO_2F_2, (d) AlNNC@Top, (e) AlNNC@Side systems

Table S1. The bond length of the most stable structures of AlNNC@SO_2, AlNNC@SOF_2, AlNNC@SO_2F_2, AlNNC@Top, and AlNNC@Side systems, along with their dipole moments.

	Bond	Bond length(Å)	Dipole Moment
AlNNC@SO_2	R_{S1-N1}	1.90	10.06
	R_{O1-Al1}	1.91	
	R_{O3-Al2}	1.94	
	R_{S2-N2}	2.02	
	R_{O2-Al3}	2.07	
	R_{O4-Al4}	2.23	
AlNNC@SOF_2	R_{F1-Al1}	1.67	12.58
	R_{F3-Al2}	1.83	
	R_{S1-N1}	1.85	
	R_{O1-Al3}	1.98	
	R_{O2-Al4}	1.87	
	R_{S2-N2}	1.74	
	R_{F2-Al5}	1.86	
	R_{F4-Al6}	1.83	
AlNNC@SO_2F_2	R_{O1-Al1}	2.01	15.58
	R_{F1-Al2}	1.91	
	R_{O2-Al3}	2.14	
AlNNC@Top	R_{F1-Al1}	1.70	26.90
	R_{S1-N1}	1.90	
	R_{O1-Al2}	1.88	
	R_{F2-Al3}	1.80	
	R_{S3-N2}	2.01	
	R_{O4-Al5}	2.09	
	R_{O2-Al4}	2.02	
AlNNC@Side	R_{O1-Al1}	1.84	12.27
	R_{F2-Al2}	1.80	
	R_{O2-Al3}	2.43	
	R_{O3-Al5}	2.01	
	R_{F1-Al6}	1.98	

The XYZ coordination of optimized pristine AlNNC with 180º disclination angle.

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Al	-1.67910	4.65890	-8.55270
N	-0.69360	5.57400	-9.92390
N	-3.45110	4.02180	-8.90920
Al	-1.65840	2.94150	-5.75200
N	-0.69000	3.96300	-7.06010
N	-3.21440	1.97190	-6.32210
Al	-4.07100	2.47480	-7.96090
Al	-4.97380	-0.65360	-8.46900
N	-5.18930	1.20910	-8.87020
N	-5.37880	-1.96210	-9.80870
Al	-1.69100	1.11060	-3.08180
N	-0.68590	2.30670	-4.21700
N	-2.51280	-0.32430	-4.06990
Al	-3.44230	0.18160	-5.66860
Al	-3.06370	-2.84870	-6.89480
N	-3.99140	-1.17170	-6.90860
N	-3.13130	-3.97230	-8.44560
Al	-4.43900	-3.63240	-9.80420
Al	0.00440	-1.07990	-1.36720
N	-0.85600	0.61220	-1.42400
N	-0.00150	-2.12320	-2.97890
Al	-1.60430	-2.02070	-4.04010
Al	-0.00930	-3.87980	-6.24540
N	-1.65140	-3.10340	-5.62500
N	-0.01080	-4.87460	-7.88410
Al	-1.66330	-5.14930	-8.81920
Al	1.69450	1.10710	-3.09230
N	0.86840	0.61000	-1.42960
N	2.50800	-0.32920	-4.08540
Al	1.59750	-2.02440	-4.04590
Al	3.04850	-2.86550	-6.89920
N	1.63740	-3.11200	-5.62700
N	3.11970	-4.00470	-8.43810
Al	1.64460	-5.17410	-8.80720
Al	1.64860	2.93780	-5.76310
N	0.68490	2.30480	-4.22170
N	3.19520	1.96200	-6.34830
Al	3.42500	0.17280	-5.69270
Al	4.93080	-0.67250	-8.50580
N	3.96730	-1.18400	-6.93160
N	5.34710	-1.99390	-9.82930
Al	4.43670	-3.68040	-9.79170
Al	1.65720	4.66720	-8.55590

N	0.67400	3.96410	-7.06260
N	3.42180	4.01950	-8.92940
Al	4.03480	2.45990	-7.99750
N	5.12990	1.18780	-8.92570
N	0.66490	5.58410	-9.92100
H	-4.50880	-4.55790	-11.05900
H	-1.65100	-5.94000	-10.16600
H	1.63160	-5.97800	-10.14610
H	4.53780	-4.63800	-11.01990
H	5.87330	-1.73700	-10.63380
H	-5.91070	-1.69990	-10.60780
H	-5.61260	1.47050	-9.73300
H	-3.88960	4.27080	-9.76760
H	-1.18410	5.92670	-10.71610
H	1.15340	5.94700	-10.70990
H	3.85590	4.27050	-9.78950
H	5.53690	1.44460	-9.79750