

Supplementary information

First theoretical framework of Al₉N₉ and B₉N₉ nanorings for unveiling their unique detection and sensing potential for SF₆ decomposition gases (H₂S, SO₂, SOF₂, and SO₂F₂): Toward real-time gas sensing in high-voltage power systems

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Partial charges:

AlN-based systems

H2S-out-AlN	SO2-out-AlN	SOF2-out-AlN	SO2F2-out-AlN
Al 0.449654	Al 0.643342	Al 0.510823	Al 0.711038
N -0.587557	N -0.537007	N -0.563061	N -0.554061
Al 0.572059	Al 0.573413	Al 0.547786	Al 0.557521
N -0.569102	N -0.567398	N -0.566919	N -0.563497
Al 0.554320	Al 0.561526	Al 0.554579	Al 0.567870
N -0.566560	N -0.564515	N -0.568108	N -0.564697
Al 0.557251	Al 0.562479	Al 0.554577	Al 0.564380
N -0.564221	N -0.563597	N -0.564783	N -0.563174
Al 0.558165	Al 0.562834	Al 0.557798	Al 0.562777
N -0.563342	N -0.563662	N -0.564028	N -0.562398
Al 0.558167	Al 0.562577	Al 0.557765	Al 0.562965
N -0.564218	N -0.564526	N -0.564877	N -0.561494
Al 0.557181	Al 0.561921	Al 0.556726	Al 0.550740
N -0.566574	N -0.567449	N -0.567980	N -0.569598
Al 0.554509	Al 0.573378	Al 0.554321	Al 0.533829
N -0.569036	N -0.537712	N -0.567826	N -0.473820
Al 0.571958	Al 0.643567	Al 0.554005	Al 0.669641
N -0.587811	N -0.524095	N -0.623538	N -0.788243
S -0.066664	S 0.854009	S 1.257890	S 1.623839
H 0.135850	O -0.554544	O -0.501931	O -0.564720
H 0.135972	O -0.554543	F -0.276755	O -0.563709
		F -0.276464	F -0.314988
			F -0.260202

BN-based systems

H2S-out-BN	SO2-out-BN	SOF2-out-BN	SO2F2-out-BN
B 0.320471	B 0.337481	B 0.302289	B 0.316485
N -0.311948	N -0.335869	N -0.316744	N -0.318941
B 0.295301	B 0.334451	B 0.316440	B 0.313347
N -0.302367	N -0.317321	N -0.318764	N -0.319518
B 0.299061	B 0.294461	B 0.304268	B 0.294626
N -0.314449	N -0.300358	N -0.305781	N -0.295812
B 0.324908	B 0.284578	B 0.299303	B 0.295648
N -0.319226	N -0.314198	N -0.316123	N -0.312789
B 0.328610	B 0.319303	B 0.304924	B 0.326523
N -0.315694	N -0.327198	N -0.315606	N -0.327713
B 0.305799	B 0.332012	B 0.298785	B 0.326075
N -0.304910	N -0.328766	N -0.305124	N -0.312277
B 0.292300	B 0.323128	B 0.304500	B 0.295307
N -0.307935	N -0.312612	N -0.319024	N -0.296169
B 0.312897	B 0.292042	B 0.316510	B 0.294873
N -0.316648	N -0.286348	N -0.316662	N -0.319281
B 0.330059	B 0.299959	B 0.302096	B 0.313319

N -0.318449	N -0.318805	N -0.294687	N -0.318922
S -0.182527	S 0.876781	S 1.174116	S 1.430377
H 0.092189	O -0.434596	O -0.489452	O -0.420128
H 0.092560	O -0.418126	F -0.312586	O -0.459419
		F -0.312679	F -0.252797
			F -0.252813

Gaussian input file:

%nprocshared=16

%mem=16GB

opt b3lyp/6-31g(d,p) empiricaldispersion=gd3

Title Card Required

0 1

Al	3.78463800	2.61270000	0.00038200
N	2.88353000	4.06035000	-0.00033600
Al	1.21967900	4.43362800	0.00066000
N	-0.40116800	4.96324900	0.00181400
Al	-1.91604300	4.18044800	0.00129800
N	-3.49834800	3.54483200	0.00085900
Al	-4.15510400	1.97118300	-0.00135400
N	-4.95818900	0.46694500	-0.00394000
Al	-4.44964100	-1.16064000	-0.00198400
N	-4.09800300	-2.82916600	-0.00041300
Al	-2.66255900	-3.74955500	0.00194200
N	-1.32084400	-4.80194000	0.00470100
Al	0.37031800	-4.58363100	0.00185000
N	2.07455700	-4.52699900	-0.00091300
Al	3.23015100	-3.27311000	-0.00190700
N	4.49938400	-2.13438900	-0.00332100
Al	4.57854400	-0.43102900	-0.00078600
N	4.81911200	1.25712900	0.00136100

S	7.39460960	2.22653614	-0.10289782
H	6.18917094	2.79577935	0.09431596
H	6.89955876	0.98013108	0.02905883