Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for:

Assessing the Efficacy of Aluminum Metal Clusters Al_{13} and Al_{15} in Mitigating NO_2 and SO_2 Pollutants: A DFT Investigation

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Table S1
The XYZ coordinates were acquired for all individualized aluminum cluster and gas structures, alongside every stable configuration of gas and cluster systems that underwent geometry optimization employing the ωB97XD/Def2-SVP method

Al_{13}			
13	-2.14527400	-0.95136600	-1.15472500
13	-0.00011800	-0.00001200	0.00020100
13	0.00363300	-0.00064000	-2.51743500
13	-1.56656000	1.74766300	-1.15410900
13	0.24270800	-2.33636900	-1.15062300
13	-2.29798300	0.49261300	1.14849500
13	-1.17985200	-2.03112200	1.15092000
13	-0.24274500	2.33635700	1.15092400
13	1.17946300	2.03115500	-1.15092300
13	2.14569700	0.95147500	1.15384100
13	1.56654600	-1.74758900	1.15435400
13	-0.00312800	0.00091300	2.51768600
13	2.29761300	-0.49307800	-1.14860500
Al_{15}			
13	-1.28501200	-0.65226400	2.06092300
13	3.14074900	-0.17107400	0.69484600
13	2.23318900	-1.72223500	-1.00748200
13	-1.29351500	0.62585600	-1.98096400
13	-4.16649400	-0.03651700	0.08968500
13	-2.02024100	-1.44089900	-0.36111100
13	1.25456200	-0.74305200	2.41846700
13	0.19927200	1.72711100	1.90608600
13	1.37227600	0.68504800	-2.23053000
13	-0.05557200	-1.71978100	-2.05691700
13	0.19842800	-2.64941800	0.65683200
13	-0.10884900	2.71590000	-0.79076100
13	-2.02034600	1.38121400	0.51171600
13	2.19471300	2.03615600	0.06304100
13	0.35684000	-0.03604500	0.02616800
NO_2			
7	-0.00000000	0.00000000	0.31740300
8	0.00000000	1.09266900	-0.13886400
8	-0.00000000	-1.09266900	-0.13886400
SO_2			
16	-0.00000000	0.00000000	0.37046000
8	0.00000000	1.24622300	-0.37046000
8	-0.00000000	-1.24622300	-0.37046000

$NO_2@Al_{13}$_1

13	-0.73719800	0.00274300	-2.54688300
13	-0.31033800	0.00017600	0.03497500
13	0.95474600	1.90020200	-1.40346800
13	-1.52780500	2.20806800	-0.97646500
13	0.95639600	-1.89789200	-1.40549600
13	-2.80638400	0.00160700	-0.95962700
13	-1.52716600	-2.20472300	-0.98366400
13	-2.30033300	1.27197400	1.36298500
13	0.20666200	2.24972300	1.26010000
13	-0.28177300	-0.00349100	2.69698900
13	0.20705000	-2.25203800	1.25434500
13	-2.29997500	-1.27728900	1.35879000
13	2.42051900	0.00155000	-0.59685400
7	4.38704600	-0.00091300	0.80064100
8	4.40452400	0.00191700	-0.45132700
8	3.20590900	-0.00210700	1.22021100

$NO_2@Al_{13}$_2

13	-1.63957100	2.03637300	1.17046000
13	-0.32464300	-0.02037200	0.00070300
13	-1.82170300	-0.37096400	2.24238200
13	-2.99307500	0.01565000	0.00491000
13	0.62869900	1.00572100	2.20788900
13	-1.64535600	1.88930400	-1.39081200
13	0.74646100	2.41712400	-0.14193000
13	-1.83271800	-0.62591300	-2.17806700
13	-1.69553300	-2.24728200	0.13289800
13	0.29977600	-1.97489700	-1.76113300
13	1.96836200	-1.42392200	0.07554900
13	0.61745800	0.74404600	-2.31389800
13	0.30926900	-1.75853000	1.97253100
7	3.85890500	0.55547300	-0.02411900
8	3.62124500	-0.79031800	0.03248900
8	4.99889700	0.81398000	-0.04629200

$NO_2@Al_{13}$_3

13	0.20795600	2.24989400	-1.25718400
13	-0.31027200	0.00006900	-0.03445300
13	2.42015300	0.00067300	0.59701000
13	0.95429100	1.89877800	1.40608600
13	-0.28023600	-0.00084200	-2.69739700
13	-1.52843100	2.20696800	0.97872500
13	-2.29898300	1.27450100	-1.36196100
13	-0.74017100	-0.00018000	2.54680900
13	0.95506000	-1.89747100	1.40710900
13	-1.52751700	-2.20703400	0.97860300
13	-2.29898600	-1.27479400	-1.36220300

13	-2.80712300	-0.00044700	0.95784500
13	0.20888100	-2.25014100	-1.25566200
7	4.38702900	-0.00026500	-0.79996100
8	4.40396200	0.00059400	0.45208200
8	3.20613000	-0.00032100	-1.22002400

$NO_2@Al_{13}$_4

13	-1.97961900	-0.00030800	-2.14070200
13	-0.52383900	-0.00030000	-0.00022600
13	-0.41522400	2.24850800	-1.41724300
13	-2.59916600	1.64062900	0.00207600
13	0.75649900	0.00135800	-2.29922400
13	-2.59727400	-1.64389300	0.00003700
13	-0.41153700	-2.24782700	-1.41862600
13	-1.97924700	-0.00060400	2.14071000
13	-0.41201400	2.24824100	1.41662500
13	0.75648400	0.00136400	2.29960400
13	1.63524300	-1.43630900	0.00002600
13	-0.41175600	-2.24754600	1.41815300
13	1.63449000	1.43619600	-0.00198500
7	4.16564800	0.00043000	0.00040400
8	3.49736600	-1.05469700	0.00009000
8	3.49650300	1.05511800	0.00081400

$NO_2@Al_{13}$_5

13	-1.65621700	1.69377600	-1.61431300
13	-0.32409300	-0.02037900	0.00276400
13	-1.63561900	2.16908600	0.90613100
13	-2.99319700	0.01479300	0.01868800
13	0.74183400	2.37973300	-0.45867600
13	-1.84493300	-0.90043200	-2.07126400
13	0.60219800	0.44037500	-2.39699200
13	-1.69177000	-2.21096300	0.42998400
13	-1.80784700	-0.08041400	2.27981400
13	0.32568600	-1.48764000	2.17782100
13	1.97011200	-1.40487900	0.24000100
13	0.28858700	-2.18614900	-1.49674100
13	0.64100900	1.28340900	2.05305200
7	3.85997600	0.55162800	-0.07838100
8	3.62239400	-0.78328800	0.10188100
8	4.99953500	0.80385100	-0.14748700

$NO_2@Al_{13}$_6

13	0.20996200	-2.24818700	-1.25864000
13	-0.30963700	0.00051600	-0.03445100
13	0.95472800	-1.90028100	1.40439300
13	2.41894600	-0.00059200	0.59623200
13	-1.52766500	-2.20911500	0.97448300

13	-0.27957400	0.00398500	-2.69744300
13	-2.29751900	-1.27256900	-1.36551400
13	0.20694600	2.25276000	-1.25351300
13	0.95458300	1.89741000	1.40800800
13	-1.52907600	2.20450100	0.98400700
13	-2.80677400	-0.00314400	0.95717200
13	-2.29950000	1.27655300	-1.35914400
13	-0.73951900	-0.00405300	2.54687100
7	4.38649200	0.00179300	-0.79921900
8	3.20564400	0.00306400	-1.21996700
8	4.40283900	-0.00103500	0.45278200

$NO_2@Al_{13}$_7

13	1.52800400	-2.20374800	0.98662100
13	0.31018900	-0.00039100	-0.03480800
13	2.80599900	0.00298100	0.96025700
13	2.30067800	-1.27751200	-1.35663700
13	0.73582300	0.00740000	2.54709800
13	-0.20632200	-2.25370000	-1.25226900
13	-0.95524900	-1.89681600	1.40854800
13	0.28321300	-0.00667700	-2.69781100
13	2.29975800	1.27186300	-1.36384800
13	-0.20836600	2.24624500	-1.26272700
13	-0.95645900	1.90368700	1.39866000
13	-2.41949900	0.00075600	0.59623000
13	1.52696100	2.20918500	0.97442400
7	-4.38670600	-0.00255300	-0.80013700
8	-3.20554200	-0.00579200	-1.22017700
8	-4.40377800	0.00271000	0.45172500

$NO_2@Al_{13}$_8

13	0.95327700	-1.89723000	-1.41036200
13	-0.30986700	0.00001800	0.03412000
13	0.21096900	-2.25098500	1.25359700
13	2.41798800	0.00035000	-0.59902500
13	-1.52869900	-2.20573100	-0.97977300
13	0.95334200	1.89949300	-1.40685900
13	-0.74246900	0.00228700	-2.54640100
13	0.21186400	2.24853900	1.25789300
13	-0.27714300	-0.00302700	2.69695500
13	-2.29615000	1.27367500	1.36542900
13	-2.80760300	0.00128400	-0.95506200
13	-1.52846400	2.20841100	-0.97538200
13	-2.29729700	-1.27594900	1.36235900
7	4.38391500	-0.00094800	0.79979000
8	3.20255500	-0.00232200	1.21881000
8	4.40192700	0.00131100	-0.45204400

$NO_2@Al_{13}$_9

13	1.83019000	-0.55694200	-2.19872300
13	0.32473000	-0.02088100	0.00016700
13	1.64508000	1.93116700	-1.33134500
13	-0.61933600	0.81798700	-2.28883000
13	2.99313700	0.01466700	0.00335500
13	-0.30194400	-1.91771000	-1.82117600
13	1.69602900	-2.25033100	0.06096800
13	-1.96906000	-1.42611300	0.03379500
13	-0.74576500	2.42035300	-0.06500500
13	-0.62701200	0.93573900	2.23875000
13	1.82325300	-0.44095800	2.22876500
13	-0.30736100	-1.82013500	1.91640900
13	1.64078300	1.99854700	1.23330200
7	-3.85881500	0.55606200	-0.01000800
8	-4.99873600	0.81560000	-0.02109800
8	-3.62172800	-0.79091200	0.01290100

$NO_2@Al_{13}$_10

13	0.60553400	0.48599200	2.40500300
13	-0.79286500	0.04953000	0.08995900
13	-2.00212200	1.18415800	2.12509100
13	-1.63077900	2.52553800	-0.14676900
13	-2.49824000	-1.39634200	1.46065600
13	0.91887900	2.18004800	0.60951400
13	0.14702600	-1.88620000	1.80013700
13	0.48961600	1.58099300	-1.76830100
13	-2.12860700	0.87974900	-2.06379000
13	0.00436200	-0.79705800	-2.38015400
13	-0.06064500	-2.53865700	-0.59532900
13	1.67420400	-0.40800200	-0.12757000
13	-2.46270300	-1.52002600	-1.19888800
7	4.28405100	0.27563400	0.00519000
8	5.40611000	-0.04900300	-0.10092800
8	3.41689700	-0.74422700	-0.24414800

$NO_2@Al_{15}$_1

13	-2.06302600	0.03129700	2.14513800
13	3.47404100	0.00019600	-0.00051400
13	1.55131600	-1.61289300	0.01941700
13	-2.06244000	-0.03128800	-2.14255200
13	-4.84298800	-0.00046200	-0.00504200
13	-2.73994700	-1.53974100	0.02418900
13	0.65046600	0.03477000	2.31367400
13	-0.59715300	2.24349000	1.37996900
13	0.65085100	-0.03355700	-2.30954100
13	-0.59825600	-2.24271500	-1.38021900
13	-0.59500100	-2.20110700	1.44568600
13	-0.59707000	2.20090500	-1.44474600

13	-2.74004500	1.53921000	-0.02191400
13	1.55106500	1.61249500	-0.02336000
13	-0.52633900	-0.00029600	0.00156500
7	5.86094900	-0.00032100	-0.00115500
8	5.14148000	-0.01457100	-1.02943500
8	5.14254300	0.01435900	1.02760100

$NO_2@Al_{15}$_2

13	0.52018500	-1.56335600	-1.82014800
13	-1.20775700	2.85279600	0.29869500
13	-2.54553700	0.82124400	0.38391300
13	1.86128600	-0.37425600	2.01608800
13	2.93281200	-3.17612700	0.17785800
13	0.60158500	-2.26356400	0.78317000
13	-1.26653400	0.50917300	-2.06589400
13	1.39485100	0.81799900	-2.46277100
13	0.60848600	1.92087700	2.07517100
13	-0.90449800	-0.42025500	2.07763700
13	-1.62678800	-1.50230400	-0.31382000
13	2.80204000	1.68404700	0.40141300
13	2.77223800	-0.68924300	-0.57922100
13	0.91590400	2.90039900	-0.94765900
13	0.34122100	0.45100300	-0.04124300
7	-4.49789200	-1.27904700	0.00332000
8	-3.50282400	-2.00500300	-0.21599300
8	-4.26069900	-0.07453300	0.24040800

$NO_2@Al_{15}$_3

13	-1.56918600	-0.88734100	-2.15456700
13	3.21072700	0.33439600	0.03697700
13	1.30610300	1.97937500	0.00684800
13	-2.49343400	0.56775000	1.77356500
13	-4.82969100	-0.57822500	-0.72340600
13	-2.84434100	1.12263500	-0.87118000
13	1.08727600	-0.57344700	-1.85687000
13	-0.17188700	-2.47823600	-0.37498300
13	0.09192100	1.01321500	2.41245500
13	-1.16384600	2.59862900	0.56230300
13	-0.48311400	1.64975300	-1.98162600
13	-0.84650900	-1.54968000	2.17380000
13	-2.63440700	-1.65663200	0.20904800
13	1.54737400	-1.14663300	1.21747900
13	-0.53176700	0.06248500	0.08646500
7	5.72302200	-0.70246000	-0.10023300
8	4.93455400	0.39984300	-0.33670000
8	6.83556600	-0.52951100	-0.41459900

$NO_2@Al_{15}$_4

13	1.15549800	1.63602600	0.00265300
13	1.07935300	-2.59407900	0.00040200
13	-0.71202700	-2.50585200	1.78480600
13	-2.94202800	0.75857100	-0.00149300
13	-1.40883200	4.07981800	0.00151900
13	-0.99219800	1.92952400	1.47268500
13	2.60379200	-0.51465300	-0.00126000
13	0.82449000	-0.08544300	-2.12097500
13	-2.72665300	-1.82814100	-0.00147500
13	-1.92899500	-0.32256900	2.29776100
13	0.82286600	-0.08852700	2.12167600
13	-1.92669100	-0.32064800	-2.29977600
13	-0.98971100	1.93126400	-1.47097700
13	-0.71040000	-2.50433300	-1.78616100
13	-0.56301100	-0.41309000	-0.00037700
7	5.23128200	0.47220500	0.00213000
8	4.68261800	1.52747200	-0.00274000
8	4.41364800	-0.57218400	0.00248900

$NO_2@Al_{15}$_5

13	0.36776700	2.65378500	-0.00217800
13	3.88645100	-0.54828900	-0.00134500
13	2.31161900	-1.26563200	1.79659100
13	-1.67477000	-1.13211500	0.00176500
13	-3.40681000	1.63050800	-0.00116000
13	-1.30742300	1.16410500	1.44472400
13	2.80580300	1.75342600	-0.00033200
13	1.24772200	1.21183900	-2.23282800
13	0.59110500	-2.56848800	0.00220300
13	-0.22958100	-1.13618700	2.21508000
13	1.24754900	1.21536900	2.23116300
13	-0.23098300	-1.13922200	-2.21260500
13	-1.30761800	1.16194400	-1.44613100
13	2.30987300	-1.26977600	-1.79583400
13	0.79036900	0.01190200	0.00004000
7	-4.57893100	-1.22146200	0.00041900
8	-3.45406900	-1.77890800	0.00207500
8	-4.56611100	0.01503700	-0.00106400

$NO_2@Al_{15}$_6

13	-1.04767100	1.59675900	-1.90768200
13	-1.70617000	-2.92876300	-0.25472700
13	0.67311700	-2.56174100	-0.69741200
13	0.82840300	0.99820500	1.87806100
13	0.46091500	4.09975200	0.05123800
13	1.25679000	1.76240700	-0.64901700
13	-1.77989300	-0.99217200	-2.20257800
13	-3.15468700	0.77835100	-0.50784200
13	0.30356700	-1.67767000	1.95027500

13	2.10676200	-0.61679400	0.24239200
13	0.82311100	-0.36750400	-2.16336100
13	-1.60610800	0.21144300	2.47315700
13	-1.28911900	2.26749200	0.74477400
13	-3.08485200	-1.29088300	0.95716100
13	-0.67595200	-0.26498600	0.02054800
7	4.06203900	-0.59506300	0.08008700
8	4.72895000	-1.54355900	0.45200300
8	4.54091900	0.41665700	-0.41642900

$NO_2@Al_{15}$_7

13	-1.10089500	0.62063400	1.83173200
13	4.82219700	0.61223200	0.73321200
13	2.84027800	-1.09087000	0.91425200
13	-0.07310800	-1.08684500	-2.38979000
13	-3.20325800	-0.33397900	-0.02771400
13	-1.30412900	-1.98825800	0.03052700
13	1.55074600	0.95181200	2.13020700
13	0.15622100	2.48369100	0.29461100
13	2.50358500	-0.61445000	-1.74543000
13	1.17293800	-2.61388400	-0.48432800
13	0.47330400	-1.59379700	2.02311100
13	0.85669800	1.48718900	-2.21809900
13	-1.54462900	1.09574500	-1.28062800
13	2.62885500	1.65499700	-0.24567800
13	0.52897600	-0.06641300	-0.08773700
7	-5.71053200	0.71573900	0.10413400
8	-6.82597100	0.54581700	0.41033400
8	-4.92745600	-0.38851700	0.34639200

$NO_2@Al_{15}$_8

13	0.54505700	1.29544400	-1.84240600
13	-0.07983100	-3.11416500	-0.60055600
13	1.14654300	-2.14840400	1.34736400
13	-1.62512700	1.18086200	1.80370900
13	-0.80245900	4.17325400	-0.13363700
13	0.61447100	2.14550600	0.66938200
13	0.90749600	-1.22907200	-2.14035500
13	-1.66313700	-0.37801600	-2.25554500
13	-1.43569300	-1.46820600	2.10754200
13	0.80504500	0.16462900	2.33818800
13	2.21577700	0.00363000	-0.04652100
13	-3.31314000	-0.08225900	0.16921500
13	-1.85355700	1.87346900	-0.84802300
13	-2.42244300	-2.32483600	-0.40272000
13	-0.43231200	-0.38432700	-0.00192000
7	4.67213800	0.21996700	-0.09935600
8	4.08247100	-0.84267600	-0.35546600
8	3.84353500	1.12550200	0.17635800

$NO_2@Al_{15}$_9

13	-2.88230000	-1.01066500	0.00086300
13	1.85239900	-2.56337700	0.00133900
13	1.36222500	-1.28097900	-2.02285400
13	-0.11033700	2.43588900	-0.00167500
13	-4.23269600	1.37915500	-0.00034800
13	-2.08319900	1.21187500	-1.41981700
13	-0.82978800	-2.76462200	0.00135100
13	-1.23601000	-1.15557900	2.20902400
13	2.13278500	0.92269100	-0.00020700
13	0.48734500	1.12523000	-2.18018000
13	-1.23663300	-1.15817800	-2.20759000
13	0.48725300	1.12806700	2.17902700
13	-2.08279600	1.21349100	1.41826100
13	1.36292000	-1.27818200	2.02390500
13	-0.16895600	-0.26223900	0.00022900
7	4.55100100	1.22493800	-0.00090600
8	3.96437800	0.11723200	-0.00125800
8	3.71739900	2.15425900	-0.00011000

$NO_2@Al_{15}$_10

13	-2.43059400	-0.00107800	-1.90772200
13	3.15310600	0.00367600	0.17921800
13	1.46363900	1.67983200	-0.69931200
13	-1.64446200	-0.00104600	2.29425900
13	-4.87057900	-0.00326000	0.78203100
13	-2.76083300	1.48868600	0.34072200
13	0.17224600	0.00095100	-2.59470100
13	-0.96207600	-2.23183700	-1.47369600
13	1.00955200	0.00097000	2.02464800
13	-0.36535100	2.22444500	1.23929100
13	-0.96623700	2.23214600	-1.47377100
13	-0.36203700	-2.22361000	1.23824200
13	-2.75869800	-1.49201400	0.33970600
13	1.46690800	-1.67574600	-0.69944300
13	-0.51997600	0.00062400	-0.09925800
7	5.84406800	-0.00639400	-0.20469000
8	6.90775700	-0.00405600	0.28417800
8	4.83869400	0.00520100	0.72332900

$SO_2@Al_{13}$_1

13	0.64587400	0.00211800	-2.22742300
13	-0.71793000	0.00000700	-0.00043800
13	-0.69025500	-2.21860900	-1.38886400
13	1.42796800	-1.39698000	0.00002300
13	-2.04483300	0.00083800	-2.23628200
13	1.42877200	1.39646300	0.00184900

13	-0.69188000	2.22028400	-1.38564000
13	0.64498500	0.00044200	2.22758900
13	-0.69201300	-2.21917300	1.38822700
13	-2.04562100	-0.00054200	2.23526000
13	-2.88214200	1.41998200	-0.00087200
13	-0.69382900	2.21844600	1.38795200
13	-2.87921700	-1.42346300	-0.00122600
16	4.18027300	0.00002200	-0.00061500
8	3.28692500	1.27595200	0.00083900
8	3.28647700	-1.27569200	0.00013800

$SO_2@Al_{13}$_2

13	-2.16719100	0.01115000	2.13214300
13	-0.66564100	-0.00020000	0.00150900
13	-2.80791200	-1.59610400	0.01595500
13	-2.80986500	1.59384400	-0.00865000
13	-0.62271900	-2.24047300	1.42990800
13	-0.63384000	2.25544000	1.40671300
13	0.56157200	0.01393200	2.31842700
13	-0.63491900	2.24078000	-1.43197400
13	-2.16751000	-0.01318100	-2.12866400
13	0.56004000	-0.01246300	-2.31555500
13	1.44114000	-1.52670900	-0.00826200
13	1.43841800	1.52986200	-0.01082000
13	-0.63917200	-2.25764200	-1.40789200
16	4.18280400	0.00123200	0.00032900
8	3.24829700	1.25209500	-0.00013400
8	3.25094300	-1.25169300	0.01111400

$SO_2@Al_{13}$_3

13	-0.38596100	2.58008400	-0.06914300
13	-0.83501300	-0.01676400	-0.00330800
13	0.15885100	0.97323900	-2.22746900
13	1.58347700	0.77046500	0.07789400
13	-2.41484400	1.43378000	-1.48264300
13	-0.01692300	1.12165200	2.22786100
13	-2.52042600	1.52332400	1.24267200
13	0.78856400	-1.42623200	1.49580800
13	0.90735900	-1.54675800	-1.21904900
13	-1.21700100	-2.60055200	0.08614300
13	-3.27214600	-0.84384700	-0.10775400
13	-1.78082900	-0.96763500	2.22808200
13	-1.56456000	-1.13667800	-2.24116700
16	4.67664700	0.19844500	-0.03159300
8	3.42012400	1.05423800	0.03931300
8	4.40194100	-1.23025600	0.01099200

$SO_2@Al_{13}$_4

13	1.26125800	1.38689100	0.29263200
13	-0.93700900	0.00011800	0.01050600
13	0.63295000	0.00216500	-1.95760300
13	1.26185700	-1.38618200	0.29029600
13	-0.79111500	2.23444700	-1.34172000
13	0.19794500	-0.00173300	2.36940600
13	-1.08291100	2.23306600	1.36674200
13	-1.08182400	-2.23525500	1.36291400
13	-0.78983300	-2.23195400	-1.34543500
13	-3.13983500	-1.38093000	-0.26476000
13	-3.14055800	1.38026000	-0.26241500
13	-2.48983900	-0.00195100	1.98961900
13	-2.06034000	0.00168500	-2.35028300
16	4.79766000	-0.00010400	-0.41029900
8	5.08471200	1.24451900	0.27966500
8	5.07875400	-1.24532800	0.28109800

$SO_2@Al_{13}$_5

13	1.40461000	-1.79396200	-0.11166700
13	-0.53283600	0.00082700	-0.00889500
13	-1.02260100	-2.62732600	-0.20611400
13	-0.14337400	-1.42335500	2.14483700
13	0.02782900	-1.11240200	-2.29789400
13	1.29870200	0.80953800	1.67143700
13	1.31745800	1.10226400	-1.45245200
13	-1.28891100	1.07924900	2.33067500
13	-2.65417900	-0.97319000	1.18063900
13	-2.65509400	1.66702400	0.12443100
13	-1.16469400	1.48597800	-2.09532600
13	-0.10260900	2.56145000	0.31771100
13	-2.52596300	-0.84091900	-1.57655900
16	3.44866100	0.23014200	0.39571100
8	3.11513800	-1.33028500	0.15068700
8	3.05524200	0.97533700	-0.97594800

$SO_2@Al_{13}$_6

13	1.43930000	-1.52782400	-0.00201600
13	-0.66654400	-0.00003300	0.00029200
13	0.56048600	0.00250200	-2.31589400
13	-0.63211900	-2.24757700	-1.42088500
13	1.43973500	1.52775800	-0.00161800
13	-0.63294800	-2.24963700	1.41749600
13	0.56156100	-0.00275000	2.31633600
13	-2.80888000	-1.59523300	-0.00164500
13	-2.16735400	0.00147400	-2.13018000
13	-2.80823100	1.59618400	0.00267400
13	-0.63004300	2.24690700	1.42151100
13	-2.16738900	-0.00143700	2.13057100
13	-0.63386800	2.25013000	-1.41732500

16	4.18227800	-0.00031500	0.00046800
8	3.24936600	1.25206500	0.00095000
8	3.24880600	-1.25218800	-0.00077900

$SO_2@Al_{13}$_7

13	1.02052700	2.62831200	0.19489400
13	0.53649500	-0.00134300	0.01072900
13	0.14625100	1.41670400	-2.14952000
13	2.65699600	0.96904700	-1.18029300
13	-1.40569600	1.79199000	0.10204100
13	2.52437400	0.85346700	1.57706100
13	-0.03058600	1.12357300	2.29317900
13	2.65474500	-1.67601900	-0.12298700
13	1.28700600	-1.08566400	-2.32694800
13	0.10017600	-2.56294900	-0.30994700
13	-1.31656200	-1.09883200	1.45664100
13	1.16771400	-1.47960000	2.09974000
13	-1.29824600	-0.81185700	-1.66502300
16	-3.44863300	-0.23264700	-0.39521300
8	-3.11759300	1.32906700	-0.15540800
8	-3.05532800	-0.97237500	0.97903600

$SO_2@Al_{13}$_8

13	1.16526500	1.47783800	2.10087100
13	0.53321600	0.00115300	0.00947800
13	-1.31688100	1.09569100	1.45857400
13	0.10394700	2.56353700	-0.30807200
13	-0.02929500	-1.12433100	2.29258500
13	2.65547500	1.66851400	-0.11877300
13	2.52499100	-0.84825100	1.57460200
13	1.29069500	1.08578600	-2.32678400
13	-1.29848600	0.82013700	-1.66751100
13	0.14217500	-1.41340000	-2.15056700
13	1.02163000	-2.62769000	0.19521800
13	2.65390800	-0.97088700	-1.18289400
13	-1.40562200	-1.79429100	0.10250200
16	-3.44825000	0.23274300	-0.39475800
8	-3.11597000	-1.32893400	-0.15702600
8	-3.05418600	0.97101500	0.98029500

$SO_2@Al_{13}$_9

13	-0.56008800	-0.00547100	-2.31681100
13	0.66525500	-0.00043600	-0.00013400
13	-1.43976800	-1.53077900	-0.00145200
13	0.63602500	-2.25212200	-1.41352900
13	-1.43892400	1.52923600	-0.00083200
13	2.16761300	-0.00683200	-2.13021300
13	0.63180300	2.24457000	-1.42476300

13	2.80888800	-1.59314800	0.00832600
13	0.63028400	-2.24423600	1.42570600
13	2.16462100	0.00692100	2.13200700
13	0.63441200	2.25198800	1.41373100
13	2.80879200	1.59323200	-0.00588900
13	-0.56349100	0.00621100	2.31475600
16	-4.18172000	0.00039200	0.00002400
8	-3.24873400	1.25247600	-0.00348700
8	-3.24914000	-1.25185300	0.00197500

$SO_2@Al_{13}$_10

13	-0.82615200	1.48114900	1.39465200
13	0.83968700	0.01646000	-0.00088600
13	1.70847600	1.02854700	2.23535900
13	-0.05100700	-1.05903200	2.23176800
13	1.22960300	2.59980800	0.01956500
13	-1.58533700	-0.75572100	0.02241800
13	-0.85750000	1.50999300	-1.32435100
13	0.37854100	-2.57851900	-0.01461300
13	2.47949900	-1.49786400	1.33533700
13	2.45125000	-1.47752900	-1.39581100
13	1.65118500	1.06749700	-2.24164300
13	-0.09816200	-1.02554000	-2.22819300
13	3.28323400	0.82854600	-0.03061700
16	-4.68830200	-0.20310400	-0.00931300
8	-3.42338700	-1.04594000	0.01064300
8	-4.43039800	1.22823100	0.00313200

$SO_2@Al_{15}$_1

13	-0.67839200	2.66605200	-0.00168700
13	-4.17370600	-0.71441500	-0.00043300
13	-2.47976800	-1.26716200	-1.76018600
13	1.51364700	-1.10714800	0.00095500
13	3.14445200	1.85345700	-0.00096900
13	1.07768900	1.23434500	-1.44041800
13	-3.06889600	1.58983500	-0.00108100
13	-1.47315300	1.21666600	2.22863200
13	-0.72409700	-2.56846400	0.00090700
13	0.06464700	-1.10557900	-2.21597200
13	-1.47345600	1.21347400	-2.22952500
13	0.06381600	-1.10430200	2.21724600
13	1.07767700	1.23576700	1.43947200
13	-2.48100000	-1.26360500	1.76175600
13	-0.94858700	0.01484100	0.00041800
16	4.68551800	-0.98926500	0.00030600
8	3.27954600	-1.64573000	0.00106300
8	4.50799900	0.54689600	-0.00023600

$SO_2@Al_{15}$_2

13	2.00715000	0.52765700	2.01891800
13	-0.68057100	-3.00371000	0.27247100
13	-2.26390800	-1.15683200	0.37373000
13	0.54184400	1.58525900	-1.81005000
13	2.75944100	3.44593300	0.20820400
13	0.54650300	2.27249500	0.79992800
13	1.00439200	-1.88597500	2.07083100
13	3.16006600	-1.39752000	0.39296200
13	-1.00528800	-0.66759300	-2.06899500
13	-1.59442200	1.30314100	-0.31637700
13	-0.75977400	0.26963700	2.07047600
13	1.68767300	-0.68084000	-2.45531900
13	2.87540900	0.96466300	-0.57177800
13	1.44335900	-2.81512900	-0.96009700
13	0.58228800	-0.44778400	-0.04396900
16	-4.62045300	0.80142100	0.00333600
8	-3.42880900	1.76102700	-0.26548300
8	-4.07454900	-0.62314700	0.28979500

$SO_2@Al_{15}$_3

13	2.00719000	0.52912400	2.01800400
13	-0.67962800	-3.00355800	0.27452600
13	-2.26379800	-1.15726800	0.37376600
13	0.54189500	1.58482300	-1.81063500
13	2.76109300	3.44508700	0.20943000
13	0.54671200	2.27255000	0.79777200
13	1.00368100	-1.88372500	2.07286600
13	3.15991200	-1.39795100	0.39474700
13	-1.00529300	-0.66826000	-2.06938300
13	-1.59496300	1.30283800	-0.31709800
13	-0.75992000	0.27091700	2.06984800
13	1.68728800	-0.68176700	-2.45582200
13	2.87467600	0.96354800	-0.57318000
13	1.44296300	-2.81510900	-0.96031200
13	0.58186600	-0.44834200	-0.04405300
16	-4.62019000	0.80198500	0.00544400
8	-4.07430300	-0.62328300	0.28810100
8	-3.42879000	1.76084100	-0.26726200

$SO_2@Al_{15}$_4

13	-0.55069400	1.64931900	-1.27360500
13	-0.43033300	-2.79858400	-1.06479600
13	2.04387600	-2.51232200	-0.95930300
13	2.61088000	0.00798200	1.82412500
13	2.10134300	3.94381700	-0.31347100
13	1.99703700	1.50835100	-1.53648900
13	-1.82788400	-0.62367100	-1.17285500
13	-1.59043600	0.88723800	1.04375500

13	1.19537200	-2.35190500	1.64346800
13	3.41007400	-0.43439700	-0.57775400
13	0.56031300	-0.56987000	-2.50284800
13	0.17542700	-0.02348900	2.68032300
13	0.83693400	2.10105600	1.09326600
13	-1.31158700	-1.78506700	1.27055700
13	0.64355500	-0.36711600	0.04109300
16	-4.44557000	0.63474600	-0.08504600
8	-3.44633200	1.21800100	0.95641900
8	-3.69132500	-0.26342000	-1.10396000

$SO_2@Al_{15}$_5

13	2.00641900	0.52911800	2.01983000
13	-0.68090900	-3.00260200	0.27079900
13	-2.26415400	-1.15632400	0.37866200
13	0.54190800	1.58301500	-1.81294600
13	2.75912500	3.44769000	0.20751200
13	0.54599300	2.27250700	0.79633200
13	1.00462900	-1.88521000	2.07173600
13	3.15998400	-1.39699800	0.39411100
13	-1.00521400	-0.67187400	-2.06726800
13	-1.59497600	1.30187000	-0.31850300
13	-0.75921100	0.27160700	2.07026800
13	1.68921300	-0.68238400	-2.45400700
13	2.87441700	0.96533900	-0.57063400
13	1.44386000	-2.81562400	-0.95978800
13	0.58244800	-0.44796700	-0.04347600
16	-4.62009900	0.80214400	0.00355700
8	-4.07460000	-0.62255700	0.28995900
8	-3.42843900	1.76100500	-0.26884500

$SO_2@Al_{15}$_6

13	-1.44188000	0.85723300	-1.29011000
13	2.91128500	0.84136900	-1.20653600
13	2.00108800	2.10343500	1.10437200
13	0.51551800	-2.08516200	1.42804100
13	-3.72197000	-2.10630100	-0.22999000
13	-1.52739500	-0.38285600	1.26307600
13	0.73131300	2.38866600	-1.30309400
13	0.69774500	-0.07779000	-2.56387000
13	2.79324700	-0.51536300	1.53028600
13	0.56466100	0.40597100	2.67229500
13	-0.65990800	2.17477800	1.00990900
13	1.90433900	-1.95983000	-0.94850600
13	-0.73850500	-1.79508000	-0.99348400
13	4.38730500	-1.13459100	-0.40282600
13	0.71093400	0.13328000	0.04494300
16	-4.11927000	0.77065400	0.08914000
8	-3.24105800	0.88037300	-1.27011900

8	-3.35304100	-0.54929000	0.90576500

$SO_2@Al_{15}$_7

13	-1.50965100	1.05398000	-0.00312500
13	3.16466000	2.13693300	-0.00087400
13	2.83377700	0.59447500	1.92126700
13	0.75268300	-2.62419800	0.00524900
13	-3.17855300	-1.84626600	-0.00026900
13	-1.12362800	-1.17756300	1.40973000
13	0.58330300	2.62434400	-0.00463600
13	0.13442700	1.06922400	-2.17484800
13	3.26813400	-1.49101700	0.00154100
13	1.34582800	-1.43653500	2.26228000
13	0.13301300	1.07629400	2.17045700
13	1.34983200	-1.44457600	-2.25624200
13	-1.12069700	-1.18355000	-1.40897100
13	2.83284000	0.59230800	-1.92112600
13	1.03896300	-0.00041400	0.00010500
16	-4.65591900	1.05537100	0.00370100
8	-4.50746600	-0.48237300	-0.00363600
8	-3.25121100	1.71354300	-0.00463900

$SO_2@Al_{15}$_8

13	1.62052200	-1.34033500	-1.94071200
13	-2.95047600	0.61363400	0.00933100
13	-1.37086400	-0.66808300	1.50467900
13	2.80298500	0.79176700	1.58214700
13	4.95128000	-1.01170500	-0.69623900
13	2.72496600	-1.70207800	0.49722100
13	-0.98882300	-0.77743400	-1.65417800
13	0.72239800	1.26005900	-2.25250300
13	0.28905700	1.55569400	2.18833100
13	1.03056800	-1.07049400	2.44487700
13	0.18475200	-2.42713800	0.16237200
13	1.57992600	2.63827000	0.02048600
13	3.08758900	0.77781300	-1.12625700
13	-0.95411100	2.12744500	-0.31269200
13	0.74245500	0.11609100	0.08551000
16	-5.91172300	-0.27287400	-0.26193600
8	-5.40602900	-1.64514800	0.01383400
8	-4.66289000	0.75519800	-0.32256900

$SO_2@Al_{15}$_9

13	2.00696600	0.52921100	-2.01921300
13	-0.67997100	-3.00322600	-0.27247100
13	1.44433800	-2.81582700	0.95924900
13	0.54162200	1.58448500	1.81205300
13	2.76025400	3.44607600	-0.20847500

13	2.87431100	0.96441400	0.57197300
13	1.00266800	-1.88400500	-2.07230300
13	-0.76003000	0.27129100	-2.06956100
13	-1.00431200	-0.67041900	2.06876300
13	1.68844400	-0.68207200	2.45449500
13	3.15988800	-1.39737900	-0.39534700
13	-1.59477100	1.30175900	0.31818600
13	0.54629700	2.27292300	-0.79722600
13	-2.26426100	-1.15719700	-0.37514300
13	0.58269400	-0.44778000	0.04387900
16	-4.62025600	0.80248500	-0.00525400
8	-3.42837200	1.76072800	0.26837500
8	-4.07533800	-0.62311200	-0.28851300

$SO_2@Al_{15}$_10

13	-1.51865900	-1.02812700	-0.00531400
13	3.13086900	-2.15208800	-0.00191100
13	2.84008300	-0.59729300	-1.92108500
13	0.76433000	2.61981000	0.00596300
13	-3.17436900	1.85426300	-0.00011700
13	-1.11377200	1.19646500	-1.41002200
13	0.55293500	-2.62865400	-0.00553400
13	0.12968000	-1.07491200	2.16847900
13	3.27271300	1.48345600	0.00412800
13	1.35778900	1.43935400	-2.25662800
13	0.13299100	-1.06591200	-2.17448800
13	1.35289200	1.42911300	2.26395500
13	-1.11670600	1.19005400	1.41089400
13	2.83953100	-0.60218000	1.92107700
13	1.04401200	-0.00748700	0.00028900
16	-4.65260300	-1.05382900	0.00203300
8	-3.24862700	-1.71630400	-0.00087400
8	-4.49943700	0.48318700	-0.00268400

Conceptual DFT

Reactivity descriptors, encompassing quantitative measures or parameters, play pivotal roles in a catalytic reaction system.[1] The utilized reactivity descriptor in this paper is based on the frontier molecular orbital (FMO) theory,[2] which includes the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). The energy disparity amid these orbitals, designated the HOMO-LUMO gap (HLG), serves as a substantial indicator of the molecule's susceptibility to undergo reactions. Furthermore, reactivity can be comprehended through descriptors such as chemical hardness and softness. Hardness, $\eta = (\varepsilon_{LUMO} - \varepsilon_{HOMO}) / 2$, gauges a molecule's resistance to electron acceptance or donation, while softness represents the opposite of hardness. These descriptors furnish insights into system stability and reactivity. The electrophilicity index (ω), elucidated by the mathematical expression $\omega = \mu^2 / (2\eta)$, encompasses the quintessence of electrophilic propensities intrinsic to a given molecular entity or atomic species within a chemical milieu. Also, the chemical potential (μ) of a system is determined based on the HOMO and the LUMO energies. The formula for the chemical potential is given by $\mu = (\varepsilon_{HOMO} + \varepsilon_{LUMO}) / 2$. The chemical potential provides insights into the energetic state of the system and serves as a fundamental parameter in various theoretical and computational analyses.[3-6]

QTAIM

The utilization of QTAIM analysis constitutes an additional potent methodology for scrutinizing the essence of interatomic interactions within a molecular framework. This technique facilitates the construction of a topological portrayal of a given molecule. Furthermore, in accordance with this theoretical framework, the spatial loci where the gradient of electron density attains a value of zero, denoted as $\nabla\rho(\mathbf{r}) = 0$, correspond to critical points in the electron density distribution. Notably, these critical points may assume the guise of either local minima, local maxima, or saddle points, and can be classified into distinct categories: (1) atomic critical points (ACP), which indicate the geometric position of an atom or nucleus (excluding hydrogen) and geometrically epitomize a local maximum point of electron density within three-dimensional space; (2) bond critical points (BCP), which demarcate critical points associated with a bond of either physical or chemical interaction, represented as saddle points featuring two directions of maximum electron density; (3) ring critical points, denoting a ring or a group of atoms that collectively constitute a ring structure, they manifest as saddle points geometrically, evincing maximum electron density along one dimension and minimum electron density along the other two dimensions; (4) cage critical points (CCP), which signify local minima points in all three dimensions of electron density. To thoroughly characterize the nature of these interactions, it becomes necessary to determine several key quantities, including the electron density ($\rho(\mathbf{r})$), the Laplacian of the electron density ($\nabla^2\rho(\mathbf{r})$), the kinetic energy density ($G(\mathbf{r})$), the potential energy density ($V(\mathbf{r})$), and the ratio of $G(\mathbf{r})$ to $V(\mathbf{r})$ denoted as $G(\mathbf{r})/V(\mathbf{r})$. A negative value of $\nabla^2\rho(\mathbf{r})$ at a bond critical point, coupled with a substantial value of $\rho(\mathbf{r})$, signifies a covalent intermolecular interaction. Conversely, if $\nabla^2\rho(\mathbf{r})$ assumes a positive value, it implies the presence of a non-substrate but closed-shell interaction, encompassing ionic and van der Waals interactions. Moreover, it is worth noting that in the case of covalent bonding, i.e., $\nabla^2\rho(\mathbf{r}) < 0$, a closed-shell interaction prevails when $\nabla^2\rho(\mathbf{r}) > 0$. Consonant with the principles of the virial theorem, the relationship of $[1/4\ \nabla^2\rho(\mathbf{r}) = 2G(\mathbf{r}) + V(\mathbf{r})]$ is established, linking $G(\mathbf{r})$, $V(\mathbf{r})$, and $\nabla^2\rho(\mathbf{r})$ within the framework of interatomic interactions. The manner of interaction can be classified based on the equilibrium between $G(\mathbf{r})$ and $V(\mathbf{r})$, with the ratio of $G(\mathbf{r})/|V(\mathbf{r})|$ serving as a suitable indicator to elucidate the nature of the interaction. A ratio less than 0.5 suggests a purely covalent form of interaction, while a ratio exceeding 1 indicates a noncovalent interaction. Based on the acquired values pertaining to each of these parameters, particularly the G/V ratio, it becomes unequivocally apparent

that the bonds delineated within Table 4 are unequivocally situated within the realm of covalent disposition. The observations elucidated in this section are in concurrence with the analyses conducted on bond order and adsorption energy.

Electron Localization Function

Greater electron localization within a region indicates a higher likelihood of confining electron motion within that specific area. Complete electron localization allows for clear differentiation from those outside the localized region. Bader observed that regions with significant electron localization exhibit large magnitudes of Fermi hole integration. However, studying the Fermi hole visually proves challenging due to its six-dimensional nature. Becke and Edgecombe proposed an alternative approach in the form of the spherically averaged like-spin conditional pair probability, which they found to have a direct correlation with the Fermi hole. Subsequently, they introduced the electron localization function (ELF) in their publication.[7]

The quantum mechanical computations produce wave functions characterized by a delocalized nature, rendering it particularly challenging to differentiate localized electronic structures from resulting electronic charges or densities. To address this inherent challenge, we advocate for the implementation of an Electron Localization Function (ELF) analysis on the distinct localized contributions within a given system.[8] The ELF function is expressed as follows: ELF = 1/ (1+ [D(r)/D0(r)] 2); The function D(r) denotes the surplus of kinetic energy density attributed to Pauli repulsion, while D0(r) represents the precise kinetic energy density of the non-interacting homogeneous electron gas, incorporated into ELF as a benchmark.[9]

The Electron Localization Function (ELF)

The Electron Localization Function (ELF) resides within the numerical interval [0, 1]. A substantial ELF value signifies pronounced electron localization, suggesting the presence of a covalent bond, a lone pair, or inner atomic shells engagement. ELF has found extensive application across diverse systems, including organic and inorganic small molecules, atomic crystals, coordination compounds, and clusters. It has been employed to address various scientific inquiries, such as elucidating atomic shell structures, classifying chemical bonding, verifying charge-shift bonds, and investigating aromaticity.

Electrostatic potential maps (ESP) and their associated contour plots have become essential tools for elucidating the relationship between molecular structures and physiochemical properties. Within the molecular framework, the combined effects of nuclei and electrons generate potentials that are currently under investigation through mapping[10]. MEP provides deeper insights into a molecule's chemical reactivity. It is closely linked to electronic density and serves as a crucial descriptor for pinpointing sites conducive to nucleophilic, electrophilic reactions, and hydrogen bonding interactions. Positive and negative regions of electrostatic potential are indicated by solid and dashed lines, respectively[11]. A vibrant array of colors vividly represents the varied values of electrostatic potential: blue signifies regions with the highest positive potential, green denotes regions of zero potential, and red indicates regions with the highest negative potential. This potential gradient follows the sequence of blue > green > yellow > red. In MEP, positive electrostatic potential arises from proton repulsion by nuclei, while negative electrostatic potential results from proton attraction by the collective electron density within the molecule. The prominent blue line corresponds to the van der Waals (vdW) surface (isosurfaces of electron density=0.001 a.u). This graphical representation confirms that the aluminum atom carries an overall positive charge, as the vdW

surface closely intersects solid contour lines surrounding it. As demonstrated in Figure 7, negative electrostatic potential predominates over the oxygen atoms, making them highly reactive sites for electrophilic attacks. Conversely, regions have blue colors used to depict the positive ESP are the most reactive sites for nucleophilic attacks. The monomer's contour maps confirm the existence of both negative and positive potential regions, consistent with the electrostatic potential map (ESP)[12]. These identified sites provide crucial information about regions where the compound can engage in intermolecular interactions

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