

Supplementary Information

Competing Plasmonic and Charge-Transfer Excitations in Pyridine Adsorbed Silver and Aluminum Nanoparticles

Junais Habeeb Mokkath

j.mokath@kcst.edu.kw

Department of Physics, Kuwait College of Science And Technology, Doha Area, 7th Ring Road, P.O.
Box 27235, Kuwait

Pyridine molecule

Atomic coordinates

C 1.628722e-16 2.128200e-01 -1.467022e+00
C 1.000000e-06 -1.014803e+00 -8.038030e-01
C -6.525180e-17 -1.031229e+00 5.877360e-01
C -1.424229e-16 1.743190e-01 1.282831e+00
C 2.000000e-06 1.370615e+00 5.644690e-01
N -2.000000e-06 1.383159e+00 -7.883220e-01
H 2.841853e-16 2.955480e-01 -2.559714e+00
H 1.524556e-16 -1.949282e+00 -1.373198e+00
H -1.254310e-16 -1.982368e+00 1.129782e+00
H -2.639027e-16 1.883280e-01 2.377024e+00
H -1.165974e-16 2.352894e+00 1.050216e+00

Ag₄₃

Atomic coordinates

Ag 1.731986e+01 1.351664e+01 1.161867e+01
Ag 1.731986e+01 1.161867e+01 1.351664e+01
Ag 1.921783e+01 1.351664e+01 1.351664e+01
Ag 1.351664e+01 1.351664e+01 1.161867e+01
Ag 1.541825e+01 1.541825e+01 1.156973e+01
Ag 1.731986e+01 1.731986e+01 1.161867e+01
Ag 1.351664e+01 1.161867e+01 1.351664e+01
Ag 1.541825e+01 1.350017e+01 1.350017e+01
Ag 1.733633e+01 1.541825e+01 1.350017e+01
Ag 1.921783e+01 1.731986e+01 1.351664e+01
Ag 1.541825e+01 1.156973e+01 1.541825e+01

Ag	1.733633e+01	1.350017e+01	1.541825e+01
Ag	1.926677e+01	1.541825e+01	1.541825e+01
Ag	1.731986e+01	1.161867e+01	1.731986e+01
Ag	1.921783e+01	1.351664e+01	1.731986e+01
Ag	1.351664e+01	1.731986e+01	1.161867e+01
Ag	1.161867e+01	1.351664e+01	1.351664e+01
Ag	1.350017e+01	1.541825e+01	1.350017e+01
Ag	1.541825e+01	1.733633e+01	1.350017e+01
Ag	1.731986e+01	1.921783e+01	1.351664e+01
Ag	1.350017e+01	1.350017e+01	1.541825e+01
Ag	1.541825e+01	1.541825e+01	1.541825e+01
Ag	1.733633e+01	1.733633e+01	1.541825e+01
Ag	1.351664e+01	1.161867e+01	1.731986e+01
Ag	1.541825e+01	1.350017e+01	1.733633e+01
Ag	1.733633e+01	1.541825e+01	1.733633e+01
Ag	1.921783e+01	1.731986e+01	1.731986e+01
Ag	1.731986e+01	1.351664e+01	1.921783e+01
Ag	1.161867e+01	1.731986e+01	1.351664e+01
Ag	1.351664e+01	1.921783e+01	1.351664e+01
Ag	1.156973e+01	1.541825e+01	1.541825e+01
Ag	1.350017e+01	1.733633e+01	1.541825e+01
Ag	1.541825e+01	1.926677e+01	1.541825e+01
Ag	1.161867e+01	1.351664e+01	1.731986e+01
Ag	1.350017e+01	1.541825e+01	1.733633e+01
Ag	1.541825e+01	1.733633e+01	1.733633e+01
Ag	1.731986e+01	1.921783e+01	1.731986e+01
Ag	1.351664e+01	1.351664e+01	1.921783e+01
Ag	1.541825e+01	1.541825e+01	1.926677e+01
Ag	1.731986e+01	1.731986e+01	1.921783e+01
Ag	1.161867e+01	1.731986e+01	1.731986e+01
Ag	1.351664e+01	1.921783e+01	1.731986e+01
Ag	1.351664e+01	1.731986e+01	1.921783e+01

Root 160

226 -> 238 : 0.034574
226 -> 239 : 0.011462
226 -> 240 : 0.022651
226 -> 241 : 0.010026
226 -> 242 : 0.016443
226 -> 244 : 0.010009
226 -> 245 : 0.014410
227 -> 238 : 0.013014
227 -> 239 : 0.010023
227 -> 240 : 0.048341
227 -> 244 : 0.027541
227 -> 246 : 0.016223
228 -> 238 : 0.010249
228 -> 243 : 0.020412
228 -> 245 : 0.037920
229 -> 248 : 0.015592
229 -> 255 : 0.022068
229 -> 256 : 0.012462
230 -> 249 : 0.031663
230 -> 250 : 0.019306
230 -> 251 : 0.020151
230 -> 252 : 0.040792
230 -> 253 : 0.022243
230 -> 257 : 0.017749
231 -> 253 : 0.025991
231 -> 256 : 0.025845
232 -> 256 : 0.034356
232 -> 257 : 0.029407
233 -> 257 : 0.010178
235 -> 251 : 0.011389

235 -> 255 : 0.011349

Root 309

219 -> 238 : 0.031493

219 -> 239 : 0.040632

220 -> 237 : 0.010676

220 -> 241 : 0.010417

221 -> 237 : 0.012333

221 -> 239 : 0.018940

222 -> 246 : 0.028521

222 -> 247 : 0.011789

222 -> 248 : 0.032684

222 -> 249 : 0.163218

222 -> 251 : 0.049641

223 -> 247 : 0.012952

223 -> 249 : 0.033803

223 -> 250 : 0.013349

223 -> 251 : 0.176603

223 -> 253 : 0.018307

236 -> 258 : 0.078637

236 -> 259 : 0.031779

236 -> 260 : 0.014052

Root 377

219 -> 246 : 0.010932

220 -> 238 : 0.011352

220 -> 248 : 0.051073

220 -> 249 : 0.017321

220 -> 251 : 0.010398

222 -> 256 : 0.047387
223 -> 256 : 0.149186
223 -> 257 : 0.035340
229 -> 259 : 0.014795
229 -> 264 : 0.012533
231 -> 261 : 0.035878
232 -> 263 : 0.029124
233 -> 260 : 0.019677
234 -> 261 : 0.011274
234 -> 262 : 0.016458
234 -> 264 : 0.018803
234 -> 267 : 0.017817
234 -> 268 : 0.021147
235 -> 263 : 0.035281
235 -> 264 : 0.016300
236 -> 262 : 0.023530
236 -> 263 : 0.010064
236 -> 265 : 0.032212
236 -> 268 : 0.016817

Root 497

226 -> 260 : 0.011664
229 -> 262 : 0.018387
229 -> 265 : 0.026162
229 -> 268 : 0.019141
229 -> 270 : 0.010882
229 -> 271 : 0.021936
230 -> 264 : 0.010548
230 -> 270 : 0.014078
231 -> 270 : 0.011261
232 -> 267 : 0.019650

232 -> 268 : 0.010436
232 -> 274 : 0.011681
232 -> 278 : 0.014444
233 -> 264 : 0.024874
233 -> 271 : 0.072648
233 -> 273 : 0.024228
233 -> 278 : 0.010704
234 -> 272 : 0.043756
234 -> 273 : 0.034144
234 -> 278 : 0.010790
235 -> 271 : 0.014388
235 -> 273 : 0.018284
235 -> 281 : 0.016600
236 -> 280 : 0.025120
236 -> 281 : 0.015445
236 -> 282 : 0.015643

Root 571

226 -> 263 : 0.012680
226 -> 267 : 0.010419
227 -> 265 : 0.014452
227 -> 269 : 0.020124
227 -> 270 : 0.013054
228 -> 262 : 0.014356
228 -> 265 : 0.011911
228 -> 269 : 0.010407
228 -> 270 : 0.076165
229 -> 272 : 0.016624
231 -> 272 : 0.010173
231 -> 275 : 0.016607
231 -> 278 : 0.014432

231 -> 280 : 0.010731
231 -> 285 : 0.022091
232 -> 277 : 0.022646
232 -> 279 : 0.016849
233 -> 274 : 0.012496
233 -> 276 : 0.012918
233 -> 278 : 0.020734
234 -> 276 : 0.010854
234 -> 279 : 0.012086
234 -> 284 : 0.012009
235 -> 275 : 0.031820
235 -> 276 : 0.019132
235 -> 280 : 0.010881
236 -> 275 : 0.013583
236 -> 280 : 0.010793
236 -> 287 : 0.022648

Ag₄₃-Pyridine (1)

Atomic coordinates

Ag	17.289560	13.119260	11.641690
Ag	17.308830	11.196640	13.521870
Ag	19.190700	13.119310	13.547750
Ag	13.535250	13.099790	11.632960
Ag	15.398390	15.041030	11.614900
Ag	17.273390	16.981890	11.644440
Ag	13.532550	11.184010	13.519400
Ag	15.406710	13.099510	13.520580

Ag	17.310120	15.047580	13.507860
Ag	19.180720	16.977120	13.532900
Ag	15.421580	11.149920	15.418470
Ag	17.301270	13.108540	15.417800
Ag	19.207920	15.055930	15.417440
Ag	17.309710	11.196800	17.314270
Ag	19.190950	13.119830	17.287740
Ag	13.490790	16.936060	11.614130
Ag	11.629590	13.083850	13.532180
Ag	13.471530	15.027370	13.504520
Ag	15.367490	16.980610	13.514590
Ag	17.288390	18.891870	13.538240
Ag	13.504430	13.088050	15.418380
Ag	15.384420	15.040370	15.417530
Ag	17.282840	16.982950	15.416950
Ag	13.532890	11.183930	17.317730
Ag	15.407350	13.099540	17.315640
Ag	17.310040	15.047940	17.327060
Ag	19.180110	16.977520	17.302040
Ag	17.290600	13.119990	19.194140
Ag	11.571540	16.915500	13.497190
Ag	13.419600	18.841540	13.480400
Ag	11.567680	15.011430	15.418260
Ag	13.430530	16.967570	15.417180
Ag	15.325560	18.873610	15.416390
Ag	11.629770	13.083820	17.304410
Ag	13.471910	15.027400	17.331220
Ag	15.367400	16.980610	17.319380
Ag	17.287690	18.891700	17.296470
Ag	13.535770	13.100000	19.203360
Ag	15.398820	15.041240	19.220590
Ag	17.272800	16.982390	19.190730
Ag	11.572610	16.916440	17.338160

Ag	13.420760	18.841570	17.354290
Ag	13.491760	16.936370	19.221430
C	16.486880	21.558140	14.234470
C	15.042000	21.474490	14.173820
C	14.291620	21.429550	15.412240
C	15.022800	21.475320	16.658040
C	16.471300	21.557610	16.618240
N	17.244130	21.617780	15.433950
H	17.089080	21.703380	13.271350
H	14.497880	21.458490	13.169890
H	13.151830	21.389390	15.403500
H	14.466930	21.460690	17.656650
H	17.058720	21.702180	17.590700

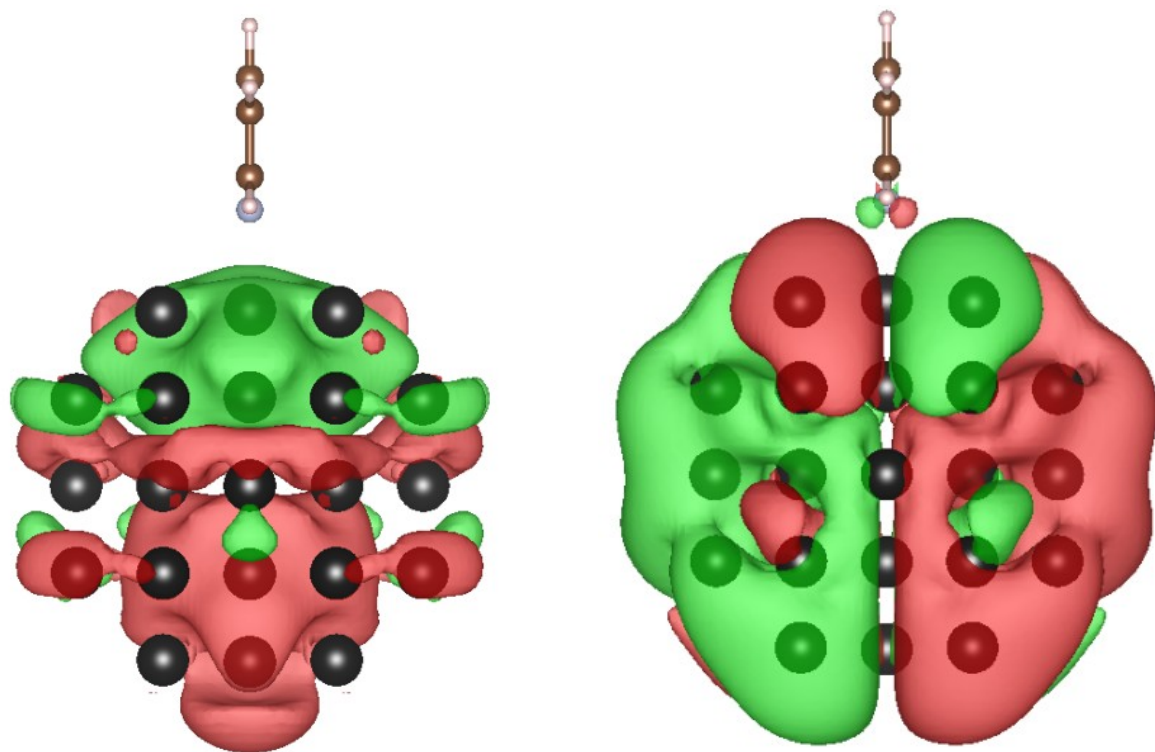


Figure S1: enlarged view of the transition density plots corresponding to the root 452 (left) and root 662 (right) as shown in Figure 4.

Orbitals

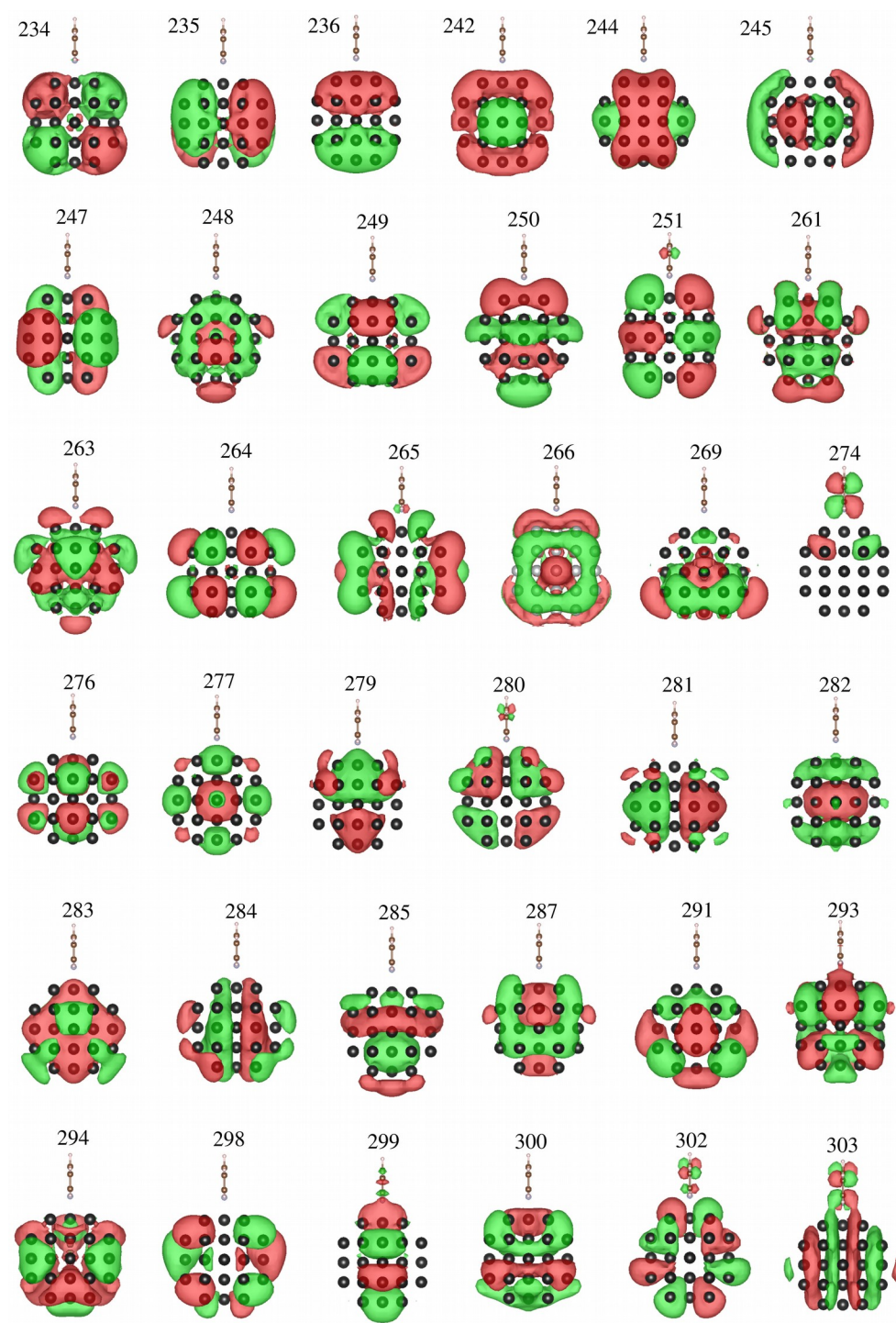


Figure S2

Natural population analysis

<u>Atoms</u>	<u>Charge</u>	<u>Valance</u>
1 ag	0.00371	10.96173
2 ag	0.03791	10.92859
3 ag	0.16217	10.80267
4 ag	0.00373	10.96172
5 ag	0.02301	10.91853
6 ag	0.02240	10.94359
7 ag	0.03790	10.92859
8 ag	-0.16861	11.04923
9 ag	-0.25202	11.13800
10 ag	0.17625	10.78957
11 ag	-0.01681	10.95827
12 ag	-0.25973	11.14297
13 ag	0.02058	10.90972
14 ag	0.03405	10.93243
15 ag	0.16419	10.80073
16 ag	0.02242	10.94357
17 ag	0.16217	10.80267
18 ag	-0.25202	11.13800
19 ag	-0.14604	11.02615
20 ag	-0.01422	10.97999
21 ag	-0.25973	11.14297
22 ag	-0.11580	10.91757
23 ag	-0.23687	11.12481
24 ag	0.03405	10.93242
25 ag	-0.15568	11.03522
26 ag	-0.25253	11.13804
27 ag	0.18033	10.78570
28 ag	0.00654	10.95895

29 ag	0.17625	10.78958
30 ag	-0.01422	10.97999
31 ag	0.02058	10.90972
32 ag	-0.23687	11.12481
33 ag	0.19294	10.72460
34 ag	0.16420	10.80073
35 ag	-0.25253	11.13804
36 ag	-0.13658	11.01545
37 ag	-0.02523	10.99127
38 ag	0.00652	10.95896
39 ag	0.02353	10.91831
40 ag	0.02564	10.94056
41 ag	0.18033	10.78570
42 ag	-0.02522	10.99127
43 ag	0.02562	10.94057
44 c	0.03726	3.94135
45 c	-0.27035	4.25792
46 c	-0.20897	4.19497
47 c	-0.27218	4.25966
48 c	0.03499	3.94350
49 n	-0.62181	5.60143
50 h	0.24085	0.75682
51 h	0.24614	0.75217
52 h	0.23990	0.75853
53 h	0.24674	0.75155
54 h	0.24114	0.75656

Root 413

234 -> 261 : 0.042526

234 -> 263 : 0.102460
234 -> 264 : 0.015573
234 -> 266 : 0.010267
235 -> 265 : 0.020550
235 -> 269 : 0.016725
236 -> 261 : 0.014301
244 -> 276 : 0.011860
244 -> 277 : 0.053311
244 -> 280 : 0.016156
245 -> 284 : 0.015843
247 -> 281 : 0.011709
247 -> 284 : 0.010819
248 -> 276 : 0.012218
249 -> 276 : 0.010253
249 -> 279 : 0.010070
249 -> 281 : 0.028813
249 -> 282 : 0.034639
249 -> 283 : 0.023127
249 -> 284 : 0.010208
249 -> 285 : 0.010739
249 -> 287 : 0.011352
250 -> 280 : 0.034100
251 -> 281 : 0.019038
251 -> 283 : 0.048996
251 -> 285 : 0.049305

Root 616

236 -> 274 : 0.020620
241 -> 286 : 0.026021
242 -> 280 : 0.012615
242 -> 284 : 0.123706
244 -> 291 : 0.011201

245 -> 302 : 0.014896
247 -> 292 : 0.010759
247 -> 293 : 0.013737
248 -> 299 : 0.033453
249 -> 294 : 0.019500
249 -> 302 : 0.052073
250 -> 298 : 0.038840
250 -> 300 : 0.112129
251 -> 302 : 0.044891
251 -> 303 : 0.013761
251 -> 305 : 0.017651

Ag₄₃-Pyridine (2)

Atomic coordinates

Ag 1.732024e+01 1.299678e+01 1.161825e+01
Ag 1.731476e+01 1.110012e+01 1.352228e+01
Ag 1.921832e+01 1.299626e+01 1.351789e+01
Ag 1.351626e+01 1.299678e+01 1.161825e+01
Ag 1.541825e+01 1.489594e+01 1.157233e+01
Ag 1.732696e+01 1.679612e+01 1.161195e+01
Ag 1.352174e+01 1.110012e+01 1.352228e+01
Ag 1.541825e+01 1.298709e+01 1.350110e+01
Ag 1.733548e+01 1.489726e+01 1.350095e+01
Ag 1.922423e+01 1.679578e+01 1.351041e+01
Ag 1.541825e+01 1.106369e+01 1.541826e+01
Ag 1.733480e+01 1.298724e+01 1.541848e+01
Ag 1.926362e+01 1.489616e+01 1.541882e+01
Ag 1.731508e+01 1.110018e+01 1.731512e+01
Ag 1.921817e+01 1.299594e+01 1.731981e+01
Ag 1.350954e+01 1.679612e+01 1.161195e+01

Ag	1.161818e+01	1.299626e+01	1.351789e+01
Ag	1.350102e+01	1.489726e+01	1.350095e+01
Ag	1.541825e+01	1.681171e+01	1.349023e+01
Ag	1.732458e+01	1.869296e+01	1.351099e+01
Ag	1.350170e+01	1.298724e+01	1.541848e+01
Ag	1.541825e+01	1.490466e+01	1.541814e+01
Ag	1.734592e+01	1.681196e+01	1.541907e+01
Ag	1.352142e+01	1.110018e+01	1.731512e+01
Ag	1.541825e+01	1.298712e+01	1.733515e+01
Ag	1.733539e+01	1.489647e+01	1.733627e+01
Ag	1.922358e+01	1.679552e+01	1.732748e+01
Ag	1.731927e+01	1.299425e+01	1.921870e+01
Ag	1.161227e+01	1.679578e+01	1.351041e+01
Ag	1.351192e+01	1.869296e+01	1.351099e+01
Ag	1.157288e+01	1.489616e+01	1.541882e+01
Ag	1.349058e+01	1.681196e+01	1.541907e+01
Ag	1.541825e+01	1.869933e+01	1.541825e+01
Ag	1.161833e+01	1.299594e+01	1.731981e+01
Ag	1.350111e+01	1.489647e+01	1.733627e+01
Ag	1.541825e+01	1.681095e+01	1.734625e+01
Ag	1.732326e+01	1.869383e+01	1.732612e+01
Ag	1.351723e+01	1.299425e+01	1.921870e+01
Ag	1.541825e+01	1.489497e+01	1.926441e+01
Ag	1.732586e+01	1.679474e+01	1.922525e+01
Ag	1.161292e+01	1.679552e+01	1.732748e+01
Ag	1.351324e+01	1.869383e+01	1.732612e+01
Ag	1.351064e+01	1.679474e+01	1.922525e+01
C	1.541825e+01	2.390633e+01	1.653228e+01
C	1.541825e+01	2.466672e+01	1.530971e+01
C	1.541825e+01	2.397763e+01	1.404655e+01
C	1.541825e+01	2.254059e+01	1.405435e+01
C	1.541825e+01	2.188223e+01	1.533079e+01
N	1.541825e+01	2.249170e+01	1.660132e+01

H	1.541825e+01	2.442856e+01	1.754814e+01
H	1.541825e+01	2.580818e+01	1.534827e+01
H	1.541825e+01	2.455201e+01	1.306037e+01
H	1.541825e+01	2.192170e+01	1.309288e+01
H	1.541825e+01	2.073122e+01	1.536105e+01

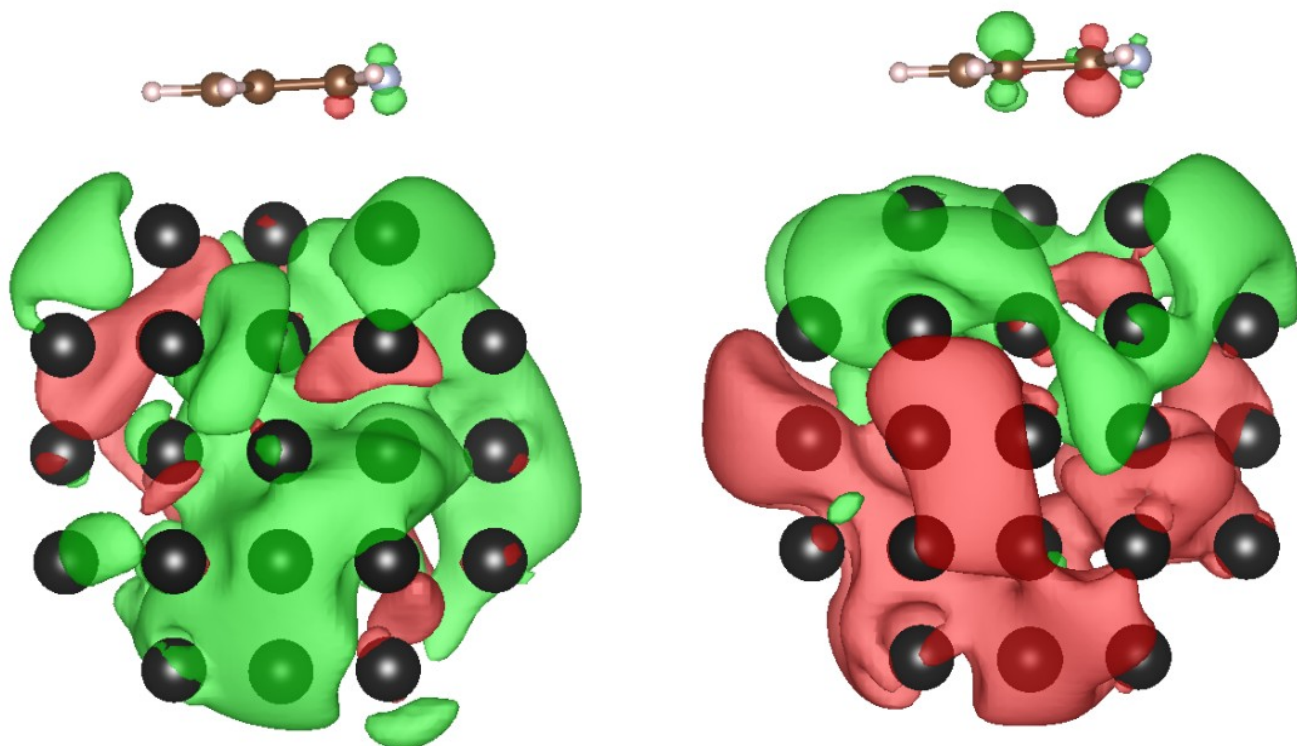


Figure S3: enlarged view of the transition density plots corresponding to the root 433 (left) and root 616 (right) as shown in Figure 6.

Orbitals

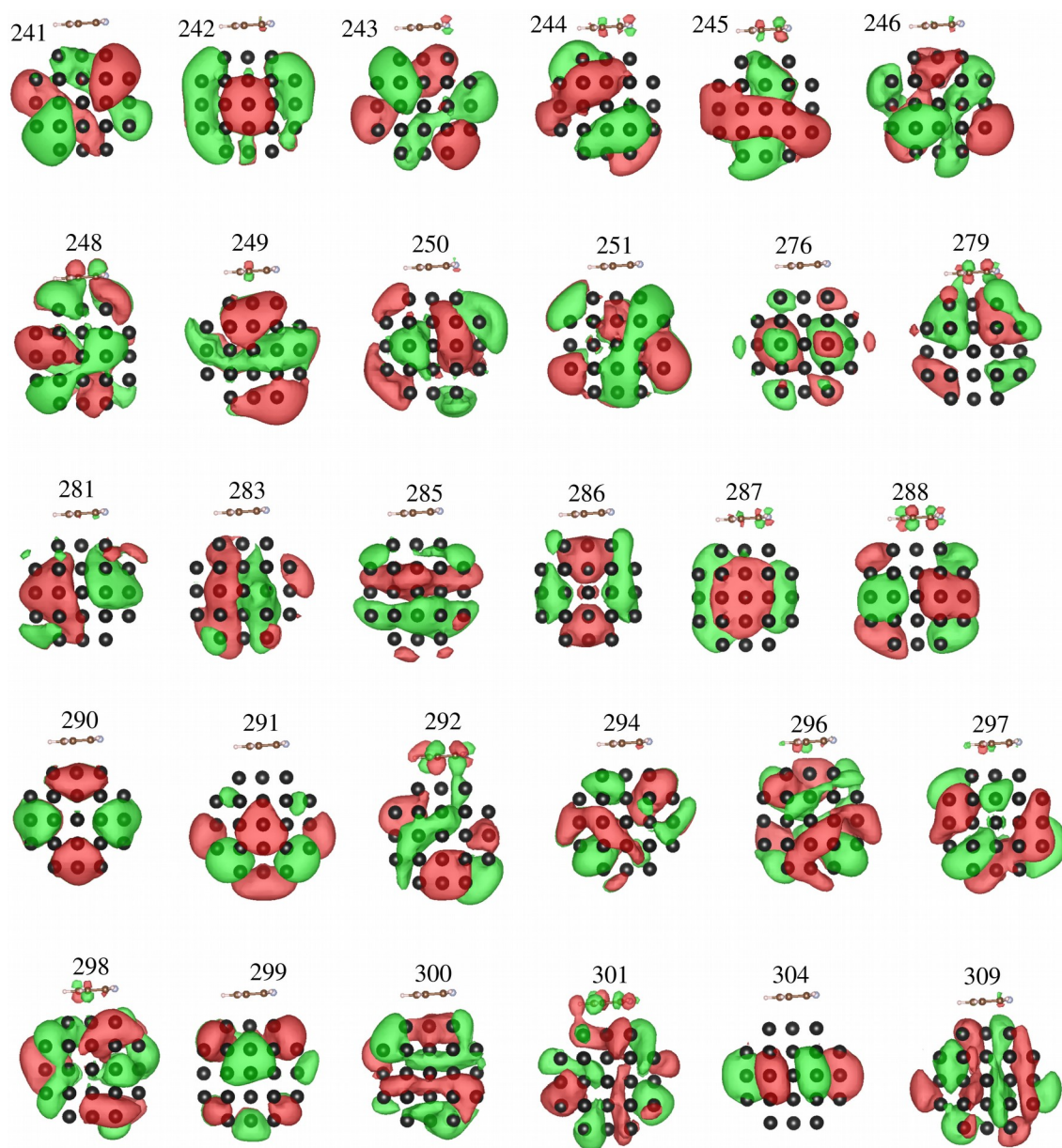


Figure S4

Root 452

242 -> 276 : 0.158672
243 -> 279 : 0.056424
243 -> 283 : 0.010225
244 -> 286 : 0.019814
244 -> 287 : 0.017558
245 -> 292 : 0.013173
246 -> 290 : 0.030788
246 -> 291 : 0.276928
248 -> 297 : 0.022359
248 -> 299 : 0.021979
248 -> 304 : 0.011682
249 -> 288 : 0.030058
250 -> 299 : 0.045779
251 -> 298 : 0.051105
251 -> 302 : 0.034193

Root 662

241 -> 285 : 0.030464
241 -> 286 : 0.023641
241 -> 287 : 0.031702
241 -> 290 : 0.056317
241 -> 291 : 0.022367
242 -> 281 : 0.028358
243 -> 296 : 0.021380
245 -> 294 : 0.019240
245 -> 300 : 0.069691
246 -> 301 : 0.153628

247 -> 300 : 0.024926
249 -> 302 : 0.105783
249 -> 306 : 0.031099
250 -> 296 : 0.019042
250 -> 298 : 0.015696
251 -> 304 : 0.020912
251 -> 309 : 0.023149
251 -> 316 : 0.010639

Al₄₃

Atomic coordinates

Al	17.319860	13.516640	11.618670
Al	17.319860	11.618670	13.516640
Al	19.217830	13.516640	13.516640
Al	13.516640	13.516640	11.618670
Al	15.418250	15.418250	11.569730
Al	17.319860	17.319860	11.618670
Al	13.516640	11.618670	13.516640
Al	15.418250	13.500170	13.500170
Al	17.336330	15.418250	13.500170
Al	19.217830	17.319860	13.516640
Al	15.418250	11.569730	15.418250
Al	17.336330	13.500170	15.418250
Al	19.266770	15.418250	15.418250
Al	17.319860	11.618670	17.319860
Al	19.217830	13.516640	17.319860
Al	13.516640	17.319860	11.618670
Al	11.618670	13.516640	13.516640

Al	13.500170	15.418250	13.500170
Al	15.418250	17.336330	13.500170
Al	17.319860	19.217830	13.516640
Al	13.500170	13.500170	15.418250
Al	15.418250	15.418250	15.418250
Al	17.336330	17.336330	15.418250
Al	13.516640	11.618670	17.319860
Al	15.418250	13.500170	17.336330
Al	17.336330	15.418250	17.336330
Al	19.217830	17.319860	17.319860
Al	17.319860	13.516640	19.217830
Al	11.618670	17.319860	13.516640
Al	13.516640	19.217830	13.516640
Al	11.569730	15.418250	15.418250
Al	13.500170	17.336330	15.418250
Al	15.418250	19.266770	15.418250
Al	11.618670	13.516640	17.319860
Al	13.500170	15.418250	17.336330
Al	15.418250	17.336330	17.336330
Al	17.319860	19.217830	17.319860
Al	13.516640	13.516640	19.217830
Al	15.418250	15.418250	19.266770
Al	17.319860	17.319860	19.217830
Al	11.618670	17.319860	17.319860
Al	13.516640	19.217830	17.319860
Al	13.516640	17.319860	19.217830

Root 17

59 -> 65 : 0.123219
59 -> 66 : 0.010776
59 -> 67 : 0.192444
59 -> 71 : 0.016918
60 -> 65 : 0.078944
60 -> 67 : 0.059917
61 -> 65 : 0.109767
61 -> 66 : 0.291522
61 -> 67 : 0.046513
61 -> 71 : 0.012685

Root 47

55 -> 68 : 0.035334
59 -> 71 : 0.204824
59 -> 72 : 0.012834
60 -> 71 : 0.036639
60 -> 72 : 0.062038
61 -> 71 : 0.134472
62 -> 69 : 0.170711
63 -> 70 : 0.069552
64 -> 69 : 0.160391

Root 92

59 -> 73 : 0.300424
59 -> 74 : 0.034588
59 -> 75 : 0.065184
60 -> 73 : 0.096281
61 -> 73 : 0.078601

61 -> 74 : 0.095553

61 -> 75 : 0.281837

Root 200

45 -> 67 : 0.066939

47 -> 72 : 0.015128

48 -> 73 : 0.012807

49 -> 75 : 0.010762

50 -> 72 : 0.034159

52 -> 71 : 0.010184

52 -> 72 : 0.116203

53 -> 68 : 0.021852

54 -> 68 : 0.010501

55 -> 68 : 0.116136

56 -> 69 : 0.065277

58 -> 69 : 0.053259

59 -> 82 : 0.018707

59 -> 83 : 0.014893

60 -> 83 : 0.033293

61 -> 81 : 0.027646

62 -> 69 : 0.011461

63 -> 76 : 0.012890

64 -> 77 : 0.018434

Root 244

50 -> 74 : 0.020896

50 -> 75 : 0.210685

51 -> 73 : 0.235844

51 -> 74 : 0.093101

51 -> 75 : 0.069001

52 -> 73 : 0.111968

52 -> 74 : 0.017773
52 -> 75 : 0.016959
55 -> 68 : 0.010421
62 -> 85 : 0.027978
62 -> 89 : 0.018618
63 -> 86 : 0.024253
63 -> 91 : 0.010515
64 -> 85 : 0.040285

Al₄₃-Pyridine (1)

Atomic coordinates

54

Al 1.731152e+01 1.294340e+01 1.162806e+01
Al 1.732147e+01 1.103086e+01 1.351545e+01
Al 1.920605e+01 1.294709e+01 1.352094e+01
Al 1.352498e+01 1.294340e+01 1.162806e+01
Al 1.541825e+01 1.486851e+01 1.161384e+01
Al 1.730858e+01 1.677752e+01 1.162424e+01
Al 1.351503e+01 1.103086e+01 1.351545e+01
Al 1.541825e+01 1.292295e+01 1.351160e+01
Al 1.732757e+01 1.486099e+01 1.350555e+01
Al 1.921362e+01 1.676404e+01 1.352177e+01
Al 1.541825e+01 1.099148e+01 1.541853e+01
Al 1.732528e+01 1.292232e+01 1.541836e+01
Al 1.922130e+01 1.486526e+01 1.541816e+01
Al 1.732145e+01 1.103123e+01 1.732164e+01
Al 1.920584e+01 1.294777e+01 1.731595e+01
Al 1.352792e+01 1.677752e+01 1.162424e+01
Al 1.163045e+01 1.294709e+01 1.352094e+01

Al	1.350893e+01	1.486099e+01	1.350555e+01
Al	1.541825e+01	1.681011e+01	1.351323e+01
Al	1.735473e+01	1.868380e+01	1.349329e+01
Al	1.351122e+01	1.292232e+01	1.541836e+01
Al	1.541825e+01	1.486778e+01	1.541785e+01
Al	1.732546e+01	1.680735e+01	1.541726e+01
Al	1.351505e+01	1.103123e+01	1.732164e+01
Al	1.541825e+01	1.292336e+01	1.732502e+01
Al	1.732721e+01	1.486164e+01	1.733052e+01
Al	1.921300e+01	1.676472e+01	1.731395e+01
Al	1.731133e+01	1.294423e+01	1.920863e+01
Al	1.162288e+01	1.676404e+01	1.352177e+01
Al	1.348177e+01	1.868380e+01	1.349329e+01
Al	1.161520e+01	1.486526e+01	1.541816e+01
Al	1.351104e+01	1.680735e+01	1.541726e+01
Al	1.541825e+01	1.873015e+01	1.541575e+01
Al	1.163066e+01	1.294777e+01	1.731595e+01
Al	1.350929e+01	1.486164e+01	1.733052e+01
Al	1.541825e+01	1.681121e+01	1.732086e+01
Al	1.735432e+01	1.868474e+01	1.733982e+01
Al	1.352517e+01	1.294423e+01	1.920863e+01
Al	1.541825e+01	1.486962e+01	1.922215e+01
Al	1.730737e+01	1.678000e+01	1.921077e+01
Al	1.162350e+01	1.676472e+01	1.731395e+01
Al	1.348218e+01	1.868474e+01	1.733982e+01
Al	1.352913e+01	1.678000e+01	1.921077e+01
C	1.541825e+01	2.135661e+01	1.662612e+01
C	1.541825e+01	2.278951e+01	1.666340e+01
C	1.541825e+01	2.352212e+01	1.542410e+01
C	1.541825e+01	2.279830e+01	1.418283e+01
C	1.541825e+01	2.136872e+01	1.420563e+01
N	1.541825e+01	2.063278e+01	1.541234e+01
H	1.541825e+01	2.070618e+01	1.756950e+01

H	1.541825e+01	2.331611e+01	1.767307e+01
H	1.541825e+01	2.466562e+01	1.543040e+01
H	1.541825e+01	2.333661e+01	1.317506e+01
H	1.541825e+01	2.072385e+01	1.325547e+01

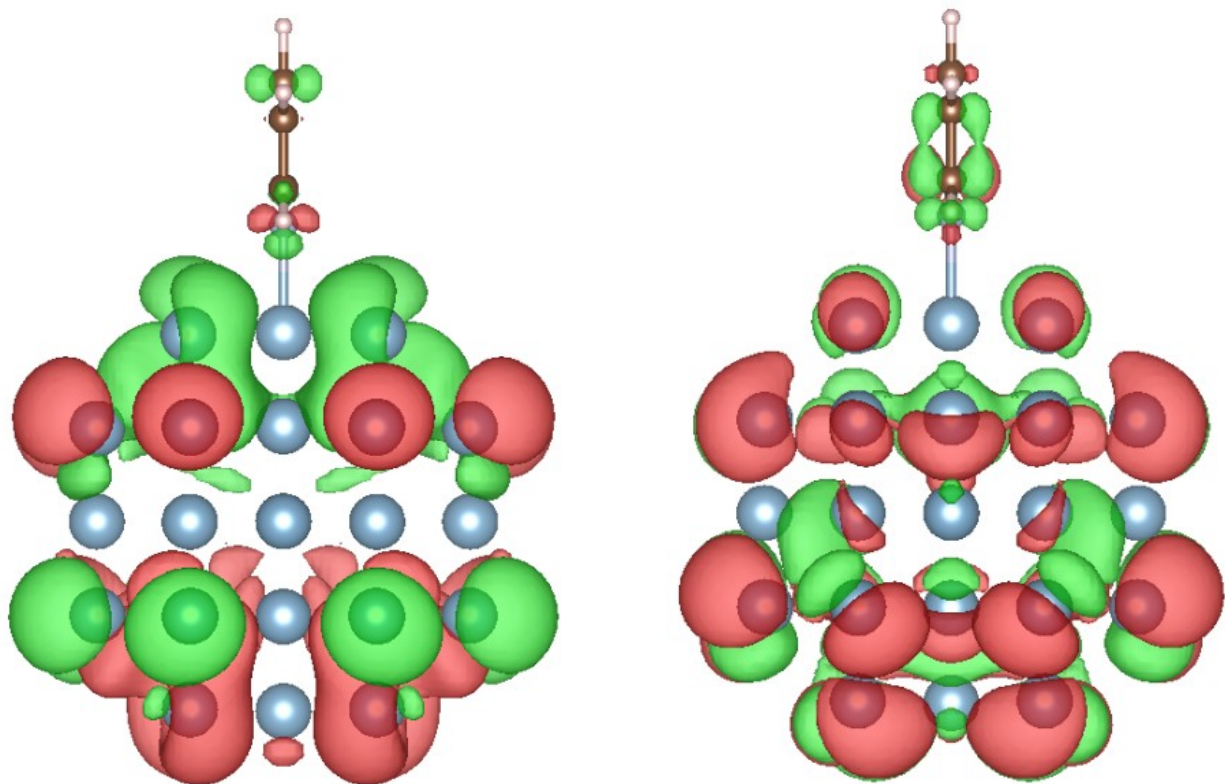


Figure S5: Enlarged view of the transition density plots corresponding to the root 138 (left) and root 212 (right) as shown in Figure 5.

Orbitals

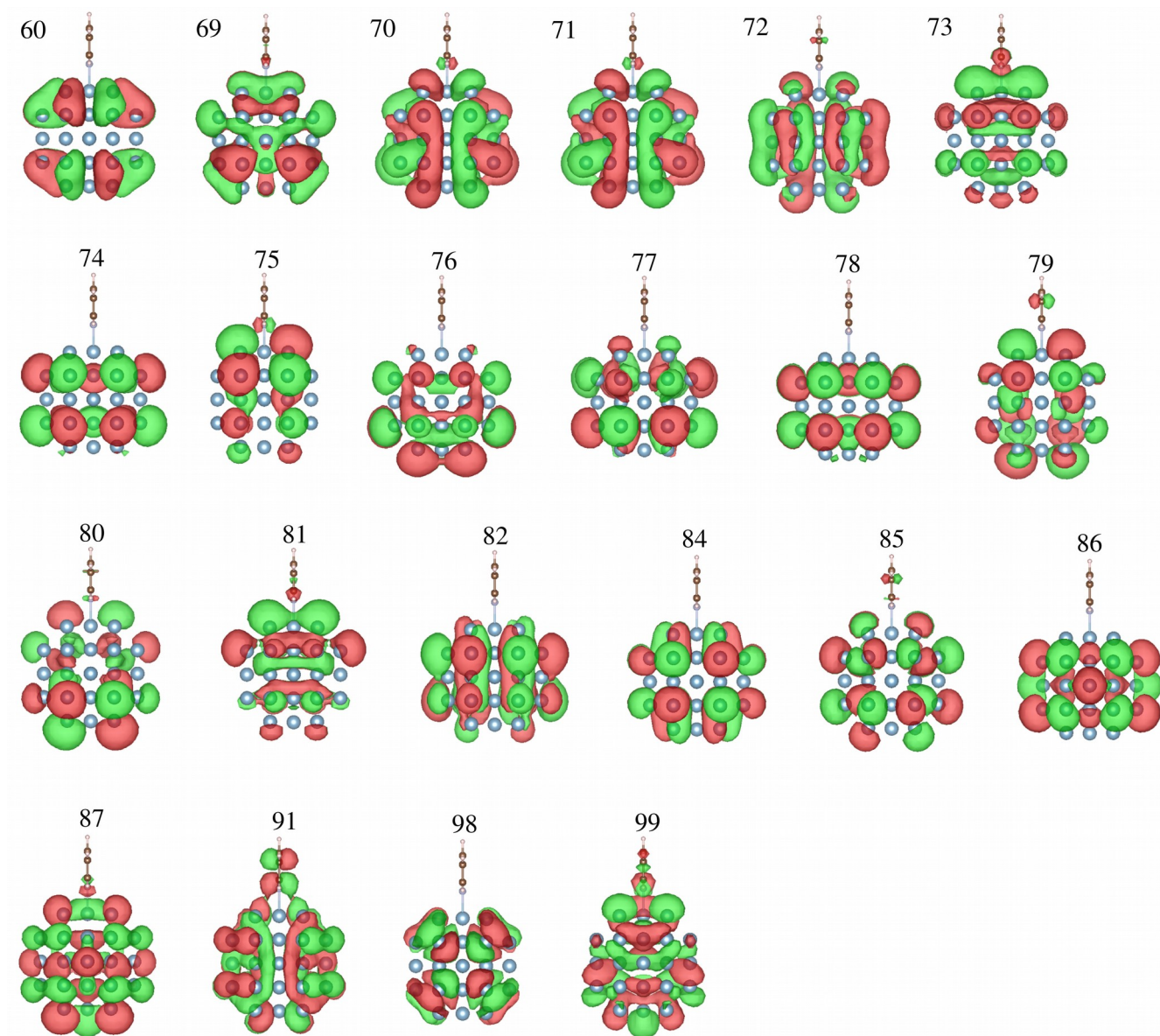


Figure S6

Root 50

69 -> 80 : 0.012199
71 -> 80 : 0.265722
72 -> 81 : 0.026724
72 -> 82 : 0.025052
72 -> 84 : 0.022725
74 -> 84 : 0.046576
74 -> 85 : 0.036804
75 -> 85 : 0.012065
75 -> 86 : 0.139388
75 -> 87 : 0.015441
76 -> 87 : 0.092550
77 -> 82 : 0.010883
77 -> 84 : 0.037998
78 -> 85 : 0.114060
79 -> 86 : 0.010125
79 -> 87 : 0.037630

Root 249

62 -> 86 : 0.137459
70 -> 91 : 0.010229
73 -> 98 : 0.039302
73 -> 102 : 0.051517
73 -> 103 : 0.010525
74 -> 99 : 0.021080
76 -> 101 : 0.011289
77 -> 99 : 0.286821
78 -> 99 : 0.205247

Al₄₃-Pyridine (2)

Atomic coordinates

Al	1.728956e+01	1.311926e+01	1.164169e+01
Al	1.730883e+01	1.119664e+01	1.352187e+01
Al	1.919070e+01	1.311931e+01	1.354775e+01
Al	1.353525e+01	1.309979e+01	1.163296e+01
Al	1.539839e+01	1.504103e+01	1.161490e+01
Al	1.727339e+01	1.698189e+01	1.164444e+01
Al	1.353255e+01	1.118401e+01	1.351940e+01
Al	1.540671e+01	1.309951e+01	1.352058e+01
Al	1.731012e+01	1.504758e+01	1.350786e+01
Al	1.918072e+01	1.697712e+01	1.353290e+01
Al	1.542158e+01	1.114992e+01	1.541847e+01
Al	1.730127e+01	1.310854e+01	1.541780e+01
Al	1.920792e+01	1.505593e+01	1.541744e+01
Al	1.730971e+01	1.119680e+01	1.731427e+01
Al	1.919095e+01	1.311983e+01	1.728774e+01
Al	1.349079e+01	1.693606e+01	1.161413e+01
Al	1.162959e+01	1.308385e+01	1.353218e+01
Al	1.347153e+01	1.502737e+01	1.350452e+01
Al	1.536749e+01	1.698061e+01	1.351459e+01
Al	1.728839e+01	1.889187e+01	1.353824e+01
Al	1.350443e+01	1.308805e+01	1.541838e+01
Al	1.538442e+01	1.504037e+01	1.541753e+01
Al	1.728284e+01	1.698295e+01	1.541695e+01
Al	1.353289e+01	1.118393e+01	1.731773e+01
Al	1.540735e+01	1.309954e+01	1.731564e+01
Al	1.731004e+01	1.504794e+01	1.732706e+01

Al	1.918011e+01	1.697752e+01	1.730204e+01
Al	1.729060e+01	1.311999e+01	1.919414e+01
Al	1.157154e+01	1.691550e+01	1.349719e+01
Al	1.341960e+01	1.884154e+01	1.348040e+01
Al	1.156768e+01	1.501143e+01	1.541826e+01
Al	1.343053e+01	1.696757e+01	1.541718e+01
Al	1.532556e+01	1.887361e+01	1.541639e+01
Al	1.162977e+01	1.308382e+01	1.730441e+01
Al	1.347191e+01	1.502740e+01	1.733122e+01
Al	1.536740e+01	1.698061e+01	1.731938e+01
Al	1.728769e+01	1.889170e+01	1.729647e+01
Al	1.353577e+01	1.310000e+01	1.920336e+01
Al	1.539882e+01	1.504124e+01	1.922059e+01
Al	1.727280e+01	1.698239e+01	1.919073e+01
Al	1.157261e+01	1.691644e+01	1.733816e+01
Al	1.342076e+01	1.884157e+01	1.735429e+01
Al	1.349176e+01	1.693637e+01	1.922143e+01
C	1.648688e+01	2.135814e+01	1.423447e+01
C	1.504200e+01	2.127449e+01	1.417382e+01
C	1.429162e+01	2.122955e+01	1.541224e+01
C	1.502280e+01	2.127532e+01	1.665804e+01
C	1.647130e+01	2.135761e+01	1.661824e+01
N	1.724413e+01	2.141778e+01	1.543395e+01
H	1.708908e+01	2.150338e+01	1.327135e+01
H	1.449788e+01	2.125849e+01	1.316989e+01
H	1.315183e+01	2.118939e+01	1.540350e+01
H	1.446693e+01	2.126069e+01	1.765665e+01
H	1.705872e+01	2.150218e+01	1.759070e+01

Orbitals

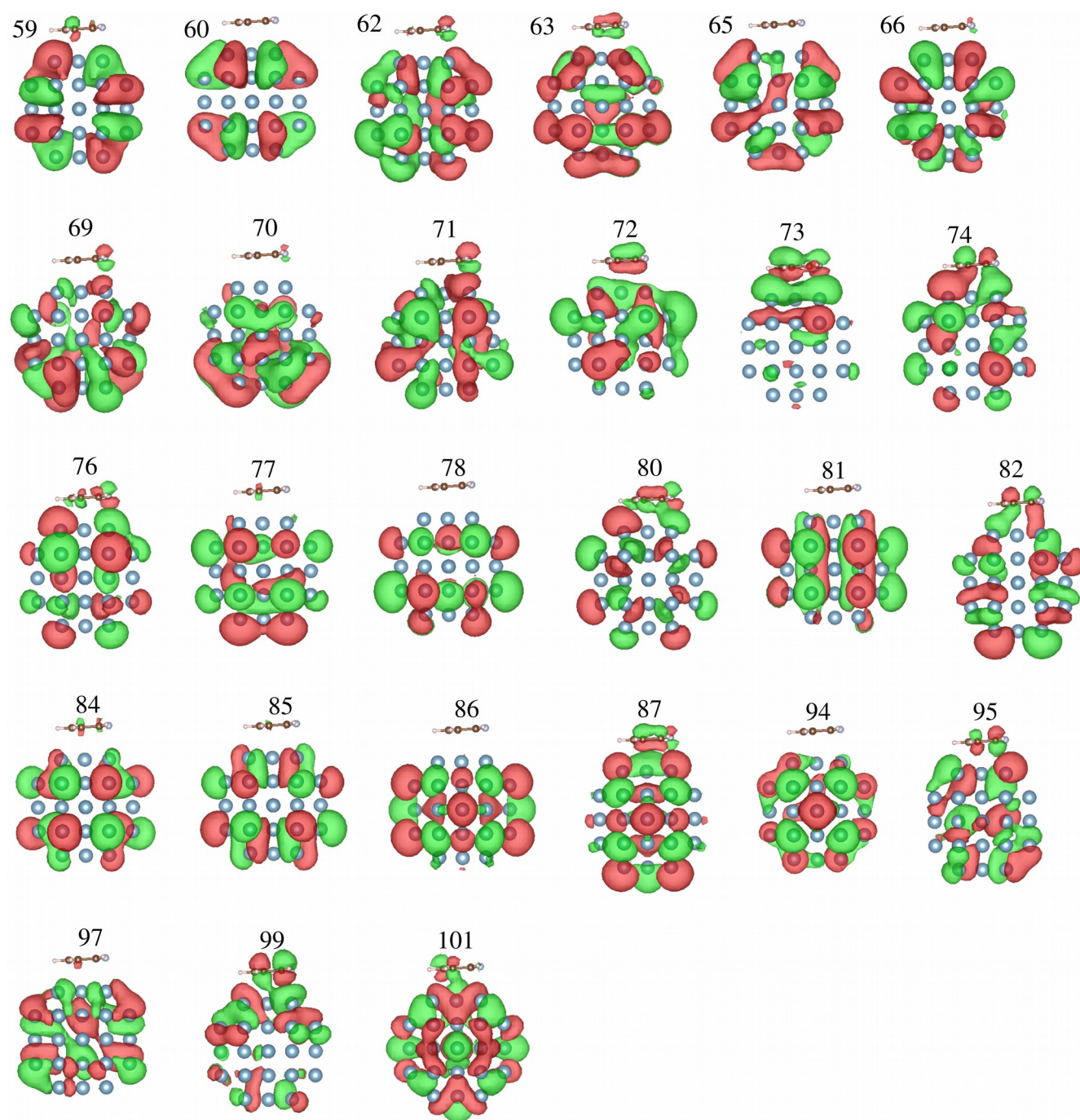


Figure S7

Root 138

60 -> 82 : 0.079268
62 -> 80 : 0.048845
62 -> 82 : 0.011322
63 -> 81 : 0.108623
65 -> 84 : 0.046566
66 -> 84 : 0.132628
69 -> 85 : 0.013642
70 -> 86 : 0.026831
71 -> 84 : 0.139084
71 -> 85 : 0.014653
72 -> 85 : 0.016108
73 -> 87 : 0.085998
77 -> 95 : 0.091243
78 -> 94 : 0.041370

Root 212

59 -> 80 : 0.024049
65 -> 85 : 0.018208
74 -> 97 : 0.065588
76 -> 99 : 0.389630
76 -> 100 : 0.130581
76 -> 101 : 0.011028
78 -> 99 : 0.113958
78 -> 100 : 0.112581

Ag₄₃ - benzene

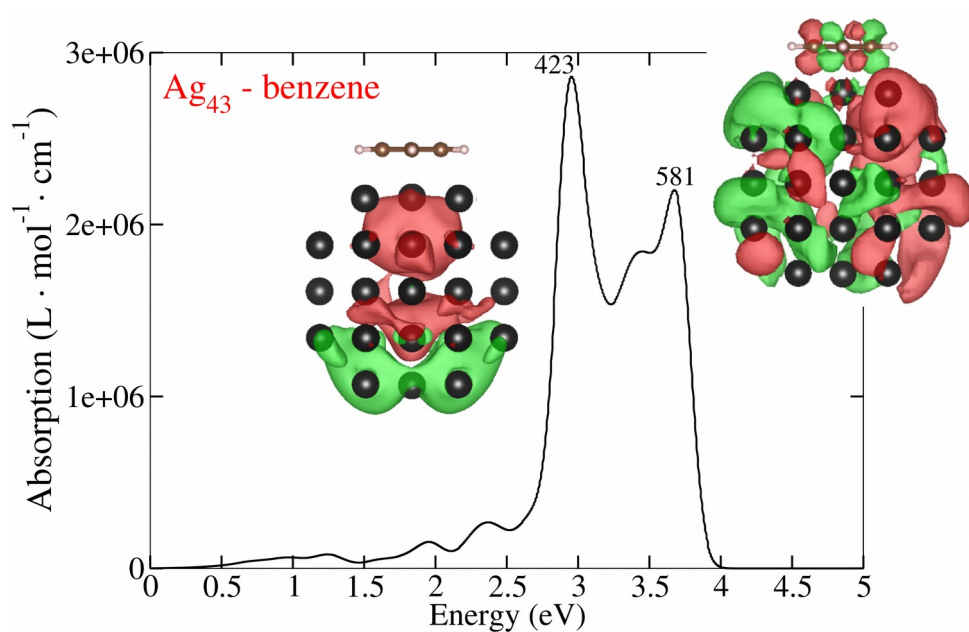


Figure S8

Al₄₃ - benzene

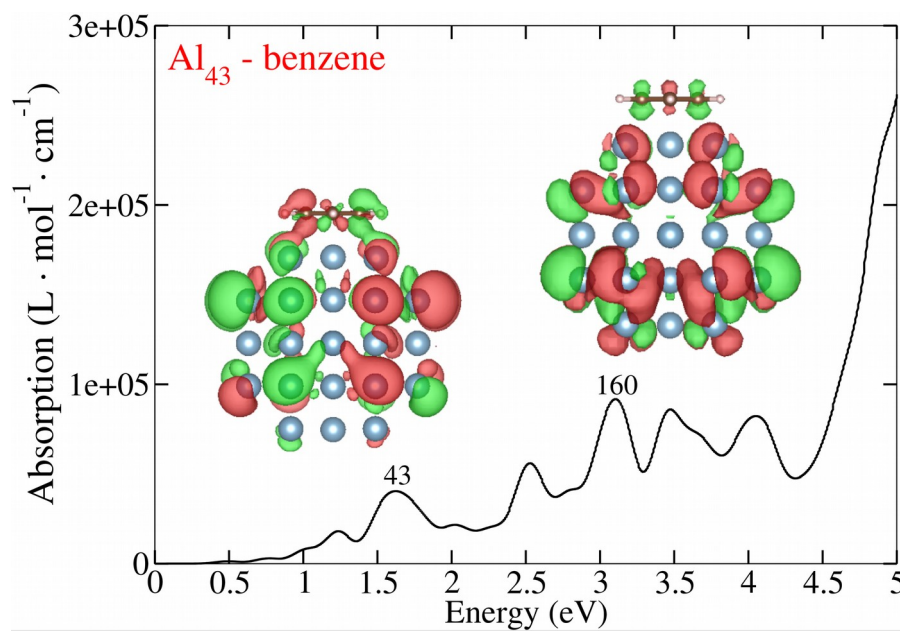


Figure S9

Al₅₅ icosahedral

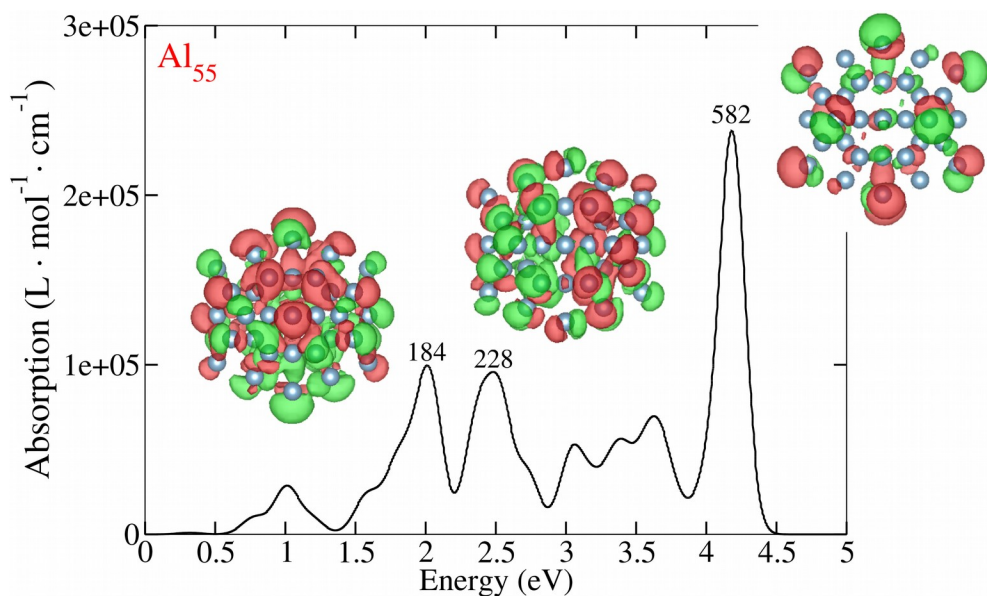


Figure S10

Al₅₅-pyridine (1)

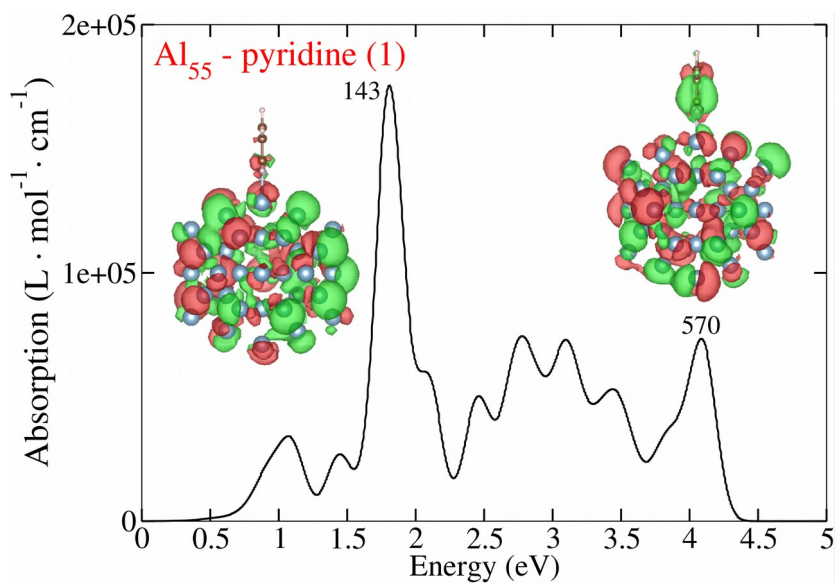


Figure S11

Al₅₅ – pyridine (2)

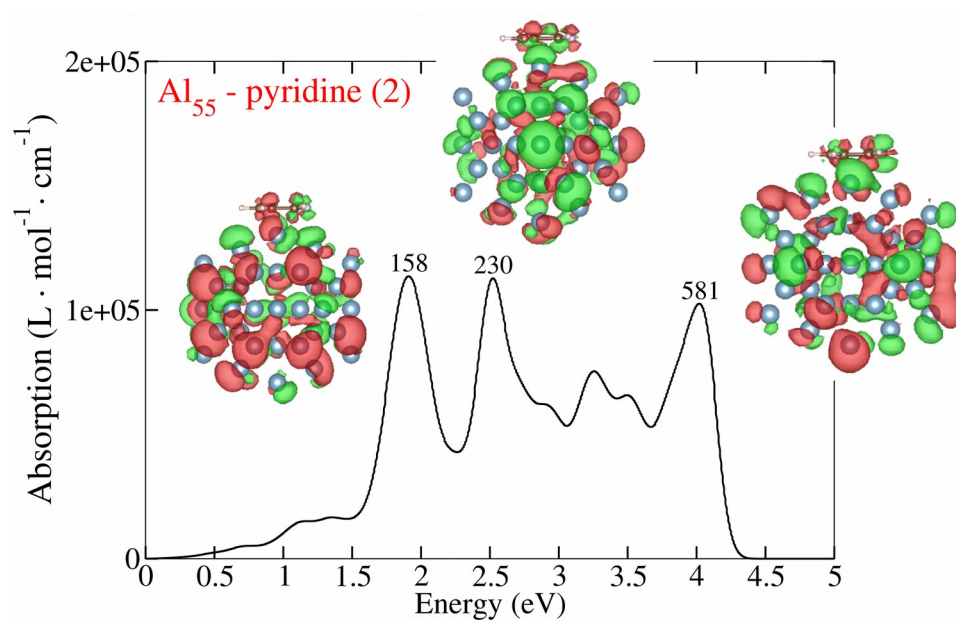


Figure S12