

SUPPORTING INFORMATION

Onset of Diradical Character in Small Nanosized Graphene Patches[†]

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S1. The total energies (in Hartree) and geometries of 4a4z, 5a5z and 6a6z in different spin states using B3LYP/6-31G(d).

System	Singlet (S=0)	Triplet (S=1)	Open-shell singlet (S=0) ^a	Heisenberg exchange coupling constant J ^b
4a4z	-1840.200073063	-1840.189947222	-1840.206601234	-0.0061
5a5z	-2681.115100440	-2681.127701868	-2681.128330905	-0.000315
6a6z	-3674.499392548	-3674.522871489	-3674.524594508	-0.00086

a – estimated for the pure open-shell singlet state^{60, 61}.

b – J is calculated from the energy differences between high spin state (S=1) and broken symmetry states⁶²⁻⁶⁴.

4a4z closed-shell singlet geometry

C	6.416232	-2.162014	0.000000
C	6.021329	-0.812489	0.000000
C	4.675128	-0.441657	0.000000
C	3.683636	-1.476130	0.000000
C	4.091169	-2.856471	0.000000
C	5.476731	-3.168133	0.000000
C	2.297695	-1.160356	0.000000
C	1.869515	0.212121	0.000000
C	2.843634	1.257628	0.000000
C	4.239047	0.957064	0.000000
C	2.408922	2.620190	0.000000
C	1.020237	2.928963	0.000000
C	0.059617	1.888329	0.000000
C	0.489435	0.521456	0.000000
C	0.588082	4.305470	0.000000
C	1.587675	5.341801	0.000000
C	2.912165	5.041172	0.000000
C	3.368267	3.677603	0.000000

C	-1.329752	2.196736	0.000000
C	-1.750024	3.575122	0.000000
C	-0.764705	4.595427	0.000000
C	-2.297695	1.160356	0.000000
C	-3.683636	1.476130	0.000000
C	-4.091169	2.856471	0.000000
C	-3.116502	3.867304	0.000000
C	-4.675128	0.441657	0.000000
C	-6.021329	0.812489	0.000000
C	-6.416232	2.162014	0.000000
C	-5.476731	3.168133	0.000000
C	5.148959	2.026933	0.000000
C	4.729386	3.349267	0.000000
C	-0.489435	-0.521456	0.000000
C	-1.869515	-0.212121	0.000000
C	-2.843634	-1.257628	0.000000
C	-4.239047	-0.957064	0.000000
C	-2.408922	-2.620190	0.000000
C	-3.368267	-3.677603	0.000000
C	-4.729386	-3.349267	0.000000
C	-5.148959	-2.026933	0.000000
C	-1.020237	-2.928963	0.000000
C	-0.059617	-1.888329	0.000000
C	1.329752	-2.196736	0.000000
C	3.116502	-3.867304	0.000000
C	1.750024	-3.575122	0.000000
C	0.764705	-4.595427	0.000000
C	-0.588082	-4.305470	0.000000
C	-1.587675	-5.341801	0.000000

C	-2.912165	-5.041172	0.000000
H	-7.475415	2.405109	0.000000
H	-5.779620	4.212178	0.000000
H	-3.438158	4.906881	0.000000
H	-1.091374	5.633553	0.000000
H	1.251424	6.375924	0.000000
H	3.657018	5.833311	0.000000
H	5.467533	4.147565	0.000000
H	6.214558	1.829704	0.000000
H	6.798309	-0.056305	0.000000
H	7.475415	-2.405109	0.000000
H	5.779620	-4.212178	0.000000
H	3.438158	-4.906881	0.000000
H	1.091374	-5.633553	0.000000
H	-1.251424	-6.375924	0.000000
H	-3.657018	-5.833311	0.000000
H	-5.467533	-4.147565	0.000000
H	-6.214558	-1.829704	0.000000
H	-6.798309	0.056305	0.000000

4a4z triplet geometry

C	6.430798	-2.142741	0.000000
C	6.042106	-0.806088	0.000000
C	4.675089	-0.435559	0.000000
C	3.695423	-1.465640	0.000000
C	4.102329	-2.845167	0.000000
C	5.480624	-3.155879	0.000000
C	2.297226	-1.149221	0.000000
C	1.878444	0.204631	0.000000

C	2.857013	1.253878	0.000000
C	4.244219	0.951013	0.000000
C	2.421912	2.617284	0.000000
C	1.030676	2.928139	0.000000
C	0.058507	1.881246	0.000000
C	0.484584	0.518595	0.000000
C	0.605011	4.290977	0.000000
C	1.592284	5.324467	0.000000
C	2.926018	5.025313	0.000000
C	3.377392	3.672160	0.000000
C	-1.322723	2.190864	0.000000
C	-1.742340	3.568267	0.000000
C	-0.769290	4.581018	0.000000
C	-2.297226	1.149221	0.000000
C	-3.695423	1.465640	0.000000
C	-4.102329	2.845167	0.000000
C	-3.122320	3.858915	0.000000
C	-4.675089	0.435559	0.000000
C	-6.042106	0.806088	0.000000
C	-6.430798	2.142741	0.000000
C	-5.480624	3.155879	0.000000
C	5.168801	2.030930	0.000000
C	4.753653	3.339836	0.000000
C	-0.484584	-0.518595	0.000000
C	-1.878444	-0.204631	0.000000
C	-2.857013	-1.253878	0.000000
C	-4.244219	-0.951013	0.000000
C	-2.421912	-2.617284	0.000000
C	-3.377392	-3.672160	0.000000

C	-4.753653	-3.339836	0.000000
C	-5.168801	-2.030930	0.000000
C	-1.030676	-2.928139	0.000000
C	-0.058507	-1.881246	0.000000
C	1.322723	-2.190864	0.000000
C	3.122320	-3.858915	0.000000
C	1.742340	-3.568267	0.000000
C	0.769290	-4.581018	0.000000
C	-0.605011	-4.290977	0.000000
C	-1.592284	-5.324467	0.000000
C	-2.926018	-5.025313	0.000000
H	-7.488415	2.392689	0.000000
H	-5.785627	4.199247	0.000000
H	-3.443393	4.898366	0.000000
H	-1.092296	5.620149	0.000000
H	1.256590	6.358759	0.000000
H	3.666979	5.821079	0.000000
H	5.487692	4.141876	0.000000
H	6.232865	1.828087	0.000000
H	6.814148	-0.045821	0.000000
H	7.488415	-2.392689	0.000000
H	5.785627	-4.199247	0.000000
H	3.443393	-4.898366	0.000000
H	1.092296	-5.620149	0.000000
H	-1.256590	-6.358759	0.000000
H	-3.666979	-5.821079	0.000000
H	-5.487692	-4.141876	0.000000
H	-6.232865	-1.828087	0.000000
H	-6.814148	0.045821	0.000000

5a5z closed-shell singlet geometry

C	5.054385	0.000000	6.512681
C	5.734511	0.000000	5.314915
C	5.022979	0.000000	4.085884
C	5.695789	0.000000	2.855872
C	5.006734	0.000000	1.635218
C	5.685061	0.000000	0.400622
C	5.001768	0.000000	-0.818255
C	5.683645	0.000000	-2.059821
C	5.004739	0.000000	-3.268821
C	5.698754	0.000000	-4.528393
C	5.019059	0.000000	-5.706017
C	2.865836	0.000000	-6.942446
C	3.584237	0.000000	-5.737388
C	2.858784	0.000000	-4.508082
C	3.564869	0.000000	-3.275207
C	2.854345	0.000000	-2.045502
C	3.559434	0.000000	-0.816241
C	2.852474	0.000000	0.417128
C	3.562086	0.000000	1.647225
C	2.861974	0.000000	2.880572
C	3.583447	0.000000	4.108810
C	2.895305	0.000000	5.359650
C	3.650245	0.000000	6.537504
C	0.691655	0.000000	6.549582
C	1.432604	0.000000	5.360384
C	0.716941	0.000000	4.127102
C	1.426496	0.000000	2.884392

C	0.717569	0.000000	1.658486
C	1.423162	0.000000	0.418881
C	0.714676	0.000000	-0.812888
C	1.421179	0.000000	-2.049488
C	0.714739	0.000000	-3.281031
C	1.427743	0.000000	-4.519893
C	0.727897	0.000000	-5.762374
C	1.482320	0.000000	-6.953158
C	-1.482320	0.000000	-6.953158
C	-0.727897	0.000000	-5.762374
C	-1.427743	0.000000	-4.519893
C	-0.714739	0.000000	-3.281031
C	-1.421179	0.000000	-2.049488
C	-0.714676	0.000000	-0.812888
C	-1.423162	0.000000	0.418881
C	-0.717569	0.000000	1.658486
C	-1.426496	0.000000	2.884392
C	-0.716941	0.000000	4.127102
C	-1.432604	0.000000	5.360384
C	-0.691655	0.000000	6.549582
C	-3.650245	0.000000	6.537504
C	-2.895305	0.000000	5.359650
C	-3.583447	0.000000	4.108810
C	-2.861974	0.000000	2.880572
C	-3.562086	0.000000	1.647225
C	-2.852474	0.000000	0.417128
C	-3.559434	0.000000	-0.816241
C	-2.854345	0.000000	-2.045502
C	-3.564869	0.000000	-3.275207

C	-2.858784	0.000000	-4.508082
C	-3.584237	0.000000	-5.737388
C	-5.019059	0.000000	-5.706017
C	-5.698754	0.000000	-4.528393
C	-5.004739	0.000000	-3.268821
C	-5.683645	0.000000	-2.059821
C	-5.685061	0.000000	0.400622
C	-5.006734	0.000000	1.635218
C	-5.695789	0.000000	2.855872
C	-5.022979	0.000000	4.085884
C	-5.734511	0.000000	5.314915
C	-5.054385	0.000000	6.512681
C	-2.865836	0.000000	-6.942446
C	-5.001768	0.000000	-0.818255
H	5.601948	0.000000	7.451303
H	6.821370	0.000000	5.290447
H	6.783893	0.000000	2.849060
H	6.773169	0.000000	0.399543
H	6.771952	0.000000	-2.057672
H	6.786077	0.000000	-4.515399
H	5.555851	0.000000	-6.651555
H	3.410462	0.000000	-7.883337
H	0.980854	0.000000	-7.913682
H	-0.980854	0.000000	-7.913682
H	-3.410462	0.000000	-7.883337
H	-5.555851	0.000000	-6.651555
H	-6.786077	0.000000	-4.515399
H	-6.771952	0.000000	-2.057672
H	-6.773169	0.000000	0.399543

H	-6.783893	0.000000	2.849060
H	-6.821370	0.000000	5.290447
H	-5.601948	0.000000	7.451303
H	-3.159818	0.000000	7.503669
H	-1.196843	0.000000	7.508239
H	1.196843	0.000000	7.508239
H	3.159818	0.000000	7.503669

5a5z triplet geometry

C	5.041885	0.000000	6.525390
C	5.724013	0.000000	5.320168
C	5.014308	0.000000	4.098181
C	5.690262	0.000000	2.859677
C	5.001859	0.000000	1.637376
C	5.680164	0.000000	0.407099
C	4.993280	0.000000	-0.826191
C	5.674751	0.000000	-2.055097
C	4.993180	0.000000	-3.276648
C	5.688916	0.000000	-4.528975
C	5.009502	0.000000	-5.711535
C	2.858091	0.000000	-6.956332
C	3.579876	0.000000	-5.743089
C	2.854373	0.000000	-4.518661
C	3.562352	0.000000	-3.281258
C	2.851057	0.000000	-2.047954
C	3.555553	0.000000	-0.822534
C	2.846582	0.000000	0.418878
C	3.555532	0.000000	1.648515
C	2.854842	0.000000	2.880331

C	3.578656	0.000000	4.119185
C	2.889932	0.000000	5.361705
C	3.645910	0.000000	6.549483
C	0.689136	0.000000	6.557798
C	1.430818	0.000000	5.362257
C	0.716219	0.000000	4.133207
C	1.427984	0.000000	2.885117
C	0.717830	0.000000	1.656797
C	1.423688	0.000000	0.421226
C	0.711667	0.000000	-0.819860
C	1.417839	0.000000	-2.051889
C	0.709857	0.000000	-3.286415
C	1.424616	0.000000	-4.530882
C	0.725214	0.000000	-5.767678
C	1.482370	0.000000	-6.967357
C	-1.482370	0.000000	-6.967357
C	-0.725214	0.000000	-5.767678
C	-1.424616	0.000000	-4.530882
C	-0.709857	0.000000	-3.286415
C	-1.417839	0.000000	-2.051889
C	-0.711667	0.000000	-0.819860
C	-1.423688	0.000000	0.421226
C	-0.717830	0.000000	1.656797
C	-1.427984	0.000000	2.885117
C	-0.716219	0.000000	4.133207
C	-1.430818	0.000000	5.362257
C	-0.689136	0.000000	6.557798
C	-3.645910	0.000000	6.549483
C	-2.889932	0.000000	5.361705

C	-3.578656	0.000000	4.119185
C	-2.854842	0.000000	2.880331
C	-3.555532	0.000000	1.648515
C	-2.846582	0.000000	0.418878
C	-3.555553	0.000000	-0.822534
C	-2.851057	0.000000	-2.047954
C	-3.562352	0.000000	-3.281258
C	-2.854373	0.000000	-4.518661
C	-3.579876	0.000000	-5.743089
C	-5.009502	0.000000	-5.711535
C	-5.688916	0.000000	-4.528975
C	-4.993180	0.000000	-3.276648
C	-5.674751	0.000000	-2.055097
C	-5.680164	0.000000	0.407099
C	-5.001859	0.000000	1.637376
C	-5.690262	0.000000	2.859677
C	-5.014308	0.000000	4.098181
C	-5.724013	0.000000	5.320168
C	-5.041885	0.000000	6.525390
C	-2.858091	0.000000	-6.956332
C	-4.993280	0.000000	-0.826191
H	5.592383	0.000000	7.462281
H	6.810920	0.000000	5.296999
H	6.778265	0.000000	2.854305
H	6.768141	0.000000	0.404648
H	6.763034	0.000000	-2.054118
H	6.776232	0.000000	-4.515310
H	5.549157	0.000000	-6.655452
H	3.406126	0.000000	-7.895271

H	0.978251	0.000000	-7.926253
H	-0.978251	0.000000	-7.926253
H	-3.406126	0.000000	-7.895271
H	-5.549157	0.000000	-6.655452
H	-6.776232	0.000000	-4.515310
H	-6.763034	0.000000	-2.054118
H	-6.768141	0.000000	0.404648
H	-6.778265	0.000000	2.854305
H	-6.810920	0.000000	5.296999
H	-5.592383	0.000000	7.462281
H	-3.151770	0.000000	7.513443
H	-1.196188	0.000000	7.515202
H	1.196188	0.000000	7.515202
H	3.151770	0.000000	7.513443

6a6z closed-shell singlet geometry

C	8.906538	-4.617595	0.000000
C	8.679678	-3.234146	0.000000
C	7.383082	-2.701609	0.000000
C	6.278037	-3.600696	0.000000
C	6.513273	-5.021469	0.000000
C	7.848104	-5.502125	0.000000
C	4.937623	-3.108547	0.000000
C	4.686861	-1.695481	0.000000
C	5.786159	-0.776652	0.000000
C	7.123882	-1.262677	0.000000
C	5.532412	0.634570	0.000000
C	4.183453	1.116189	0.000000
C	3.100580	0.200402	0.000000

C	3.355843	-1.213356	0.000000
C	3.927106	2.523515	0.000000
C	5.017743	3.452221	0.000000
C	6.360190	2.988064	0.000000
C	6.618811	1.555574	0.000000
C	4.750978	4.858367	0.000000
C	3.411603	5.333759	0.000000
C	2.330029	4.413492	0.000000
C	2.592335	3.000461	0.000000
C	3.148643	6.749314	0.000000
C	4.264027	7.656509	0.000000
C	5.543822	7.196923	0.000000
C	5.829916	5.791011	0.000000
C	0.997161	4.888808	0.000000
C	0.738951	6.307741	0.000000
C	1.835973	7.200736	0.000000
C	-0.092764	3.971254	0.000000
C	-1.423494	4.448691	0.000000
C	-1.677347	5.873475	0.000000
C	-0.586317	6.761259	0.000000
C	-2.513158	3.534533	0.000000
C	-3.850554	4.015607	0.000000
C	-4.096404	5.441894	0.000000
C	-3.004138	6.327713	0.000000
C	-4.937623	3.108547	0.000000
C	-6.278037	3.600696	0.000000
C	-6.513273	5.021469	0.000000
C	-5.420509	5.902087	0.000000
C	-7.383082	2.701609	0.000000

C	-8.679678	3.234146	0.000000
C	-8.906538	4.617595	0.000000
C	-7.848104	5.502125	0.000000
C	7.401199	3.941605	0.000000
C	7.145819	5.299758	0.000000
C	1.504139	2.082173	0.000000
C	0.163027	2.561604	0.000000
C	-0.922989	1.647381	0.000000
C	-2.262308	2.128197	0.000000
C	-3.355843	1.213356	0.000000
C	-4.686861	1.695481	0.000000
C	-5.786159	0.776652	0.000000
C	-7.123882	1.262677	0.000000
C	-5.532412	-0.634570	0.000000
C	-6.618811	-1.555574	0.000000
C	-7.924530	-1.035718	0.000000
C	-8.167064	0.322863	0.000000
C	-4.183453	-1.116189	0.000000
C	-3.100580	-0.200402	0.000000
C	-1.759220	-0.678703	0.000000
C	-0.667936	0.238678	0.000000
C	0.667936	-0.238678	0.000000
C	1.759220	0.678703	0.000000
C	8.167064	-0.322863	0.000000
C	7.924530	1.035718	0.000000
C	2.262308	-2.128197	0.000000
C	0.922989	-1.647381	0.000000
C	-0.163027	-2.561604	0.000000
C	-1.504139	-2.082173	0.000000

C	-2.592335	-3.000461	0.000000
C	-3.927106	-2.523515	0.000000
C	-5.017743	-3.452221	0.000000
C	-6.360190	-2.988064	0.000000
C	-4.750978	-4.858367	0.000000
C	-5.829916	-5.791011	0.000000
C	-7.145819	-5.299758	0.000000
C	-7.401199	-3.941605	0.000000
C	-3.411603	-5.333759	0.000000
C	-2.330029	-4.413492	0.000000
C	-0.997161	-4.888808	0.000000
C	0.092764	-3.971254	0.000000
C	1.423494	-4.448691	0.000000
C	2.513158	-3.534533	0.000000
C	3.850554	-4.015607	0.000000
C	5.420509	-5.902087	0.000000
C	4.096404	-5.441894	0.000000
C	3.004138	-6.327713	0.000000
C	1.677347	-5.873475	0.000000
C	0.586317	-6.761259	0.000000
C	-0.738951	-6.307741	0.000000
C	-1.835973	-7.200736	0.000000
C	-3.148643	-6.749314	0.000000
C	-4.264027	-7.656509	0.000000
C	-5.543822	-7.196923	0.000000
H	-9.927547	4.988930	0.000000
H	-8.021148	6.574771	0.000000
H	-5.607785	6.972777	0.000000
H	-3.196593	7.397593	0.000000

H	-0.780737	7.830891	0.000000
H	1.637286	8.269619	0.000000
H	4.059366	8.723935	0.000000
H	6.380753	7.891043	0.000000
H	7.975247	6.003263	0.000000
H	8.434319	3.614251	0.000000
H	8.777944	1.703683	0.000000
H	9.198130	-0.656666	0.000000
H	9.540762	-2.576095	0.000000
H	9.927547	-4.988930	0.000000
H	8.021148	-6.574771	0.000000
H	5.607785	-6.972777	0.000000
H	3.196593	-7.397593	0.000000
H	0.780737	-7.830891	0.000000
H	-1.637286	-8.269619	0.000000
H	-4.059366	-8.723935	0.000000
H	-6.380753	-7.891043	0.000000
H	-7.975247	-6.003263	0.000000
H	-8.434319	-3.614251	0.000000
H	-8.777944	-1.703683	0.000000
H	-9.198130	0.656666	0.000000
H	-9.540762	2.576095	0.000000

6a6z triplet geometry

C	8.912438	-4.611581	0.000000
C	8.685705	-3.232291	0.000000
C	7.385328	-2.700023	0.000000
C	6.283761	-3.599305	0.000000
C	6.520397	-5.016646	0.000000

C	7.849898	-5.497781	0.000000
C	4.937997	-3.106410	0.000000
C	4.688432	-1.696037	0.000000
C	5.789972	-0.776450	0.000000
C	7.126122	-1.262256	0.000000
C	5.536172	0.634082	0.000000
C	4.185443	1.115714	0.000000
C	3.102240	0.200112	0.000000
C	3.357536	-1.213605	0.000000
C	3.929440	2.520966	0.000000
C	5.022356	3.450674	0.000000
C	6.362846	2.986681	0.000000
C	6.621250	1.555026	0.000000
C	4.756274	4.855534	0.000000
C	3.414152	5.331395	0.000000
C	2.333642	4.410696	0.000000
C	2.595333	2.997797	0.000000
C	3.152905	6.743504	0.000000
C	4.265026	7.651346	0.000000
C	5.546371	7.192267	0.000000
C	5.832305	5.788076	0.000000
C	1.000850	4.886689	0.000000
C	0.745743	6.301753	0.000000
C	1.834799	7.194366	0.000000
C	-0.092188	3.968410	0.000000
C	-1.421056	4.445965	0.000000
C	-1.672938	5.870100	0.000000
C	-0.589432	6.756128	0.000000
C	-2.513584	3.531694	0.000000

C	-3.852585	4.012574	0.000000
C	-4.099789	5.438945	0.000000
C	-3.006547	6.326077	0.000000
C	-4.937997	3.106410	0.000000
C	-6.283761	3.599305	0.000000
C	-6.520397	5.016646	0.000000
C	-5.420822	5.900463	0.000000
C	-7.385328	2.700023	0.000000
C	-8.685705	3.232291	0.000000
C	-8.912438	4.611581	0.000000
C	-7.849898	5.497781	0.000000
C	7.405989	3.941526	0.000000
C	7.150980	5.297045	0.000000
C	1.506704	2.079967	0.000000
C	0.163250	2.559784	0.000000
C	-0.921624	1.646867	0.000000
C	-2.263725	2.128316	0.000000
C	-3.357536	1.213605	0.000000
C	-4.688432	1.696037	0.000000
C	-5.789972	0.776450	0.000000
C	-7.126122	1.262256	0.000000
C	-5.536172	-0.634082	0.000000
C	-6.621250	-1.555026	0.000000
C	-7.928512	-1.035379	0.000000
C	-8.170962	0.321859	0.000000
C	-4.185443	-1.115714	0.000000
C	-3.102240	-0.200112	0.000000
C	-1.761161	-0.678794	0.000000
C	-0.666980	0.239047	0.000000

C	0.666980	-0.239047	0.000000
C	1.761161	0.678794	0.000000
C	8.170962	-0.321859	0.000000
C	7.928512	1.035379	0.000000
C	2.263725	-2.128316	0.000000
C	0.921624	-1.646867	0.000000
C	-0.163250	-2.559784	0.000000
C	-1.506704	-2.079967	0.000000
C	-2.595333	-2.997797	0.000000
C	-3.929440	-2.520966	0.000000
C	-5.022356	-3.450674	0.000000
C	-6.362846	-2.986681	0.000000
C	-4.756274	-4.855534	0.000000
C	-5.832305	-5.788076	0.000000
C	-7.150980	-5.297045	0.000000
C	-7.405989	-3.941526	0.000000
C	-3.414152	-5.331395	0.000000
C	-2.333642	-4.410696	0.000000
C	-1.000850	-4.886689	0.000000
C	0.092188	-3.968410	0.000000
C	1.421056	-4.445965	0.000000
C	2.513584	-3.531694	0.000000
C	3.852585	-4.012574	0.000000
C	5.420822	-5.900463	0.000000
C	4.099789	-5.438945	0.000000
C	3.006547	-6.326077	0.000000
C	1.672938	-5.870100	0.000000
C	0.589432	-6.756128	0.000000
C	-0.745743	-6.301753	0.000000

C	-1.834799	-7.194366	0.000000
C	-3.152905	-6.743504	0.000000
C	-4.265026	-7.651346	0.000000
C	-5.546371	-7.192267	0.000000
H	-9.932739	4.984801	0.000000
H	-8.023156	6.570675	0.000000
H	-5.607438	6.971502	0.000000
H	-3.197910	7.396146	0.000000
H	-0.781914	7.826130	0.000000
H	1.637093	8.263682	0.000000
H	4.060328	8.718897	0.000000
H	6.382588	7.887209	0.000000
H	7.977847	6.003272	0.000000
H	8.438684	3.613712	0.000000
H	8.780615	1.704662	0.000000
H	9.201636	-0.656168	0.000000
H	9.545325	-2.572496	0.000000
H	9.932739	-4.984801	0.000000
H	8.023156	-6.570675	0.000000
H	5.607438	-6.971502	0.000000
H	3.197910	-7.396146	0.000000
H	0.781914	-7.826130	0.000000
H	-1.637093	-8.263682	0.000000
H	-4.060328	-8.718897	0.000000
H	-6.382588	-7.887209	0.000000
H	-7.977847	-6.003272	0.000000
H	-8.438684	-3.613712	0.000000
H	-8.780615	-1.704662	0.000000
H	-9.201636	0.656168	0.000000

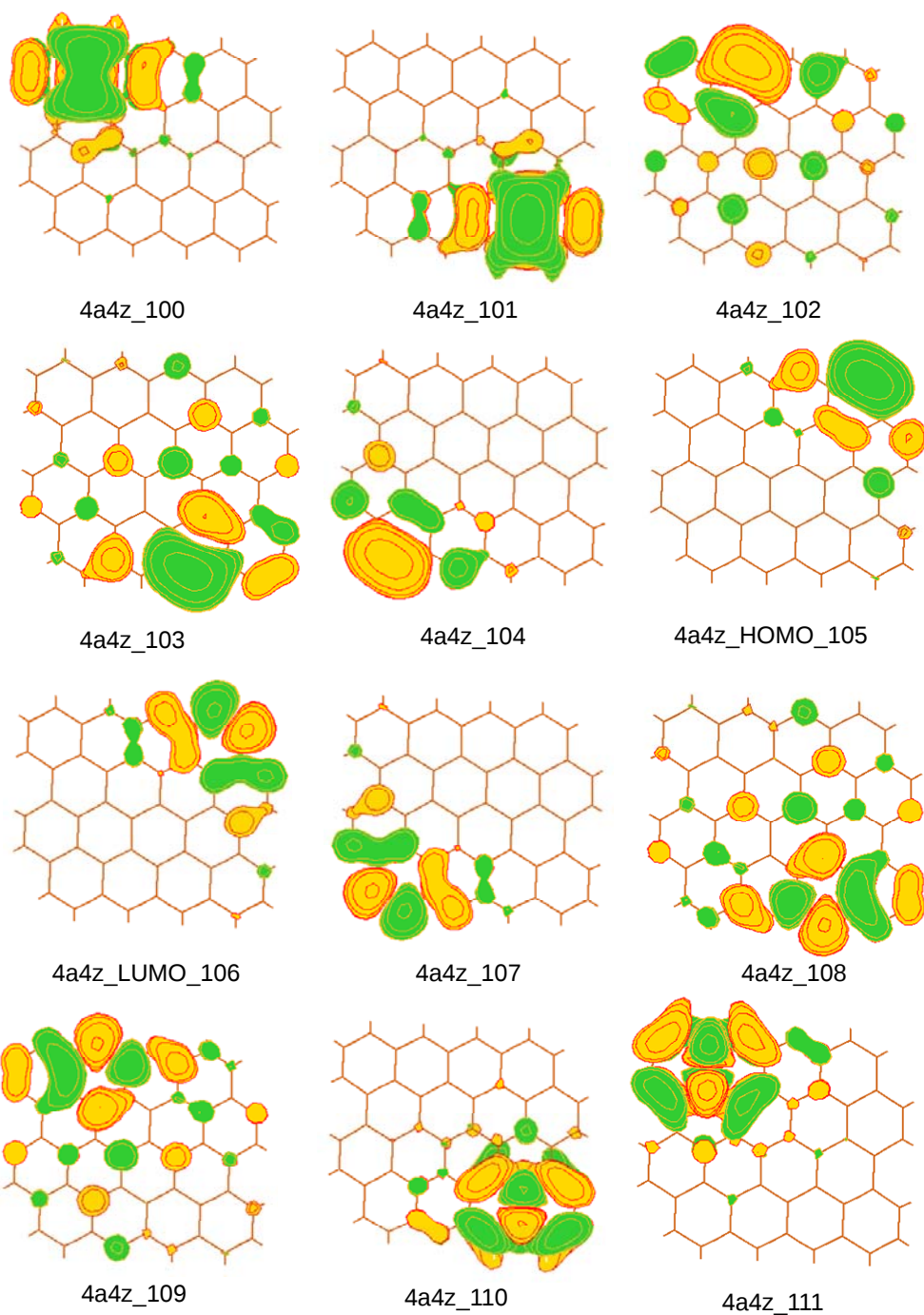
H	-9.545325	2.572496	0.000000
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S2. The orbital occupation numbers of PP calculations using SBKJC-ECP with sto-3G level.

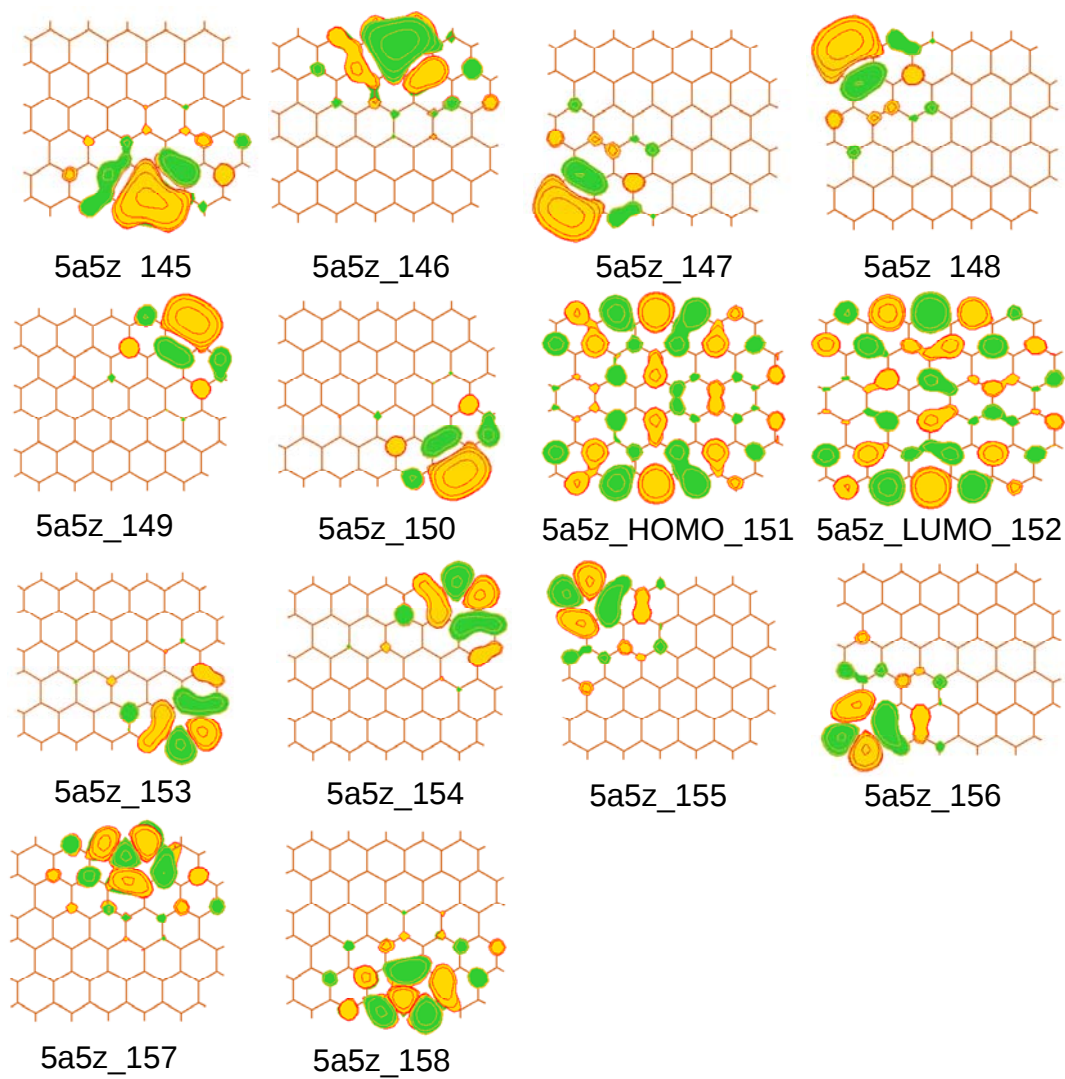
Bolds represent the HOMO and LUMO for different system..

4a4z	alpha	beta	5a5z	alpha	beta	6a6z	alpha	beta
			145	0.98612	0.98612			
100	0.98845	0.98845	146	0.98612	0.98612			
101	0.98845	0.98845	147	0.9667	0.9667	201	0.97686	0.97686
102	0.96627	0.96627	148	0.9667	0.9667	202	0.97686	0.97686
103	0.96627	0.96627	149	0.95464	0.95464	203	0.96837	0.96837
104	0.94824	0.94824	150	0.95464	0.95464	204	0.96837	0.96837
105	0.94824	0.94824	151	0.62432	0.62432	205	0.52304	0.52304
106	0.05176	0.05176	152	0.37568	0.37568	206	0.47696	0.47696
107	0.05176	0.05176	153	0.04536	0.04536	207	0.03163	0.03163
108	0.03373	0.03373	154	0.04536	0.04536	208	0.03163	0.03163
109	0.03373	0.03373	155	0.0333	0.0333	209	0.02314	0.02314
110	0.01155	0.01155	156	0.0333	0.0333	210	0.02314	0.02314
111	0.01155	0.01155	157	0.01388	0.01388			
			158	0.01388	0.01388			
			5a6z	alpha	beta	6a5z	alpha	beta
						171	0.98006	0.98006
			172	0.98193	0.98193	172	0.97812	0.97812
			173	0.97685	0.97685	173	0.96318	0.96318
			174	0.96795	0.96795	174	0.96288	0.96288
			175	0.96746	0.96746	175	0.95799	0.95799
			176	0.54854	0.54854	176	0.95756	0.95756
			177	0.45146	0.45146	177	0.04244	0.04244
			178	0.03254	0.03254	178	0.04201	0.04201
			179	0.03205	0.03205	179	0.03712	0.03712
			180	0.02315	0.02315	180	0.03682	0.03682
			181	0.01807	0.01807	181	0.02188	0.02188
						182	0.01994	0.01994

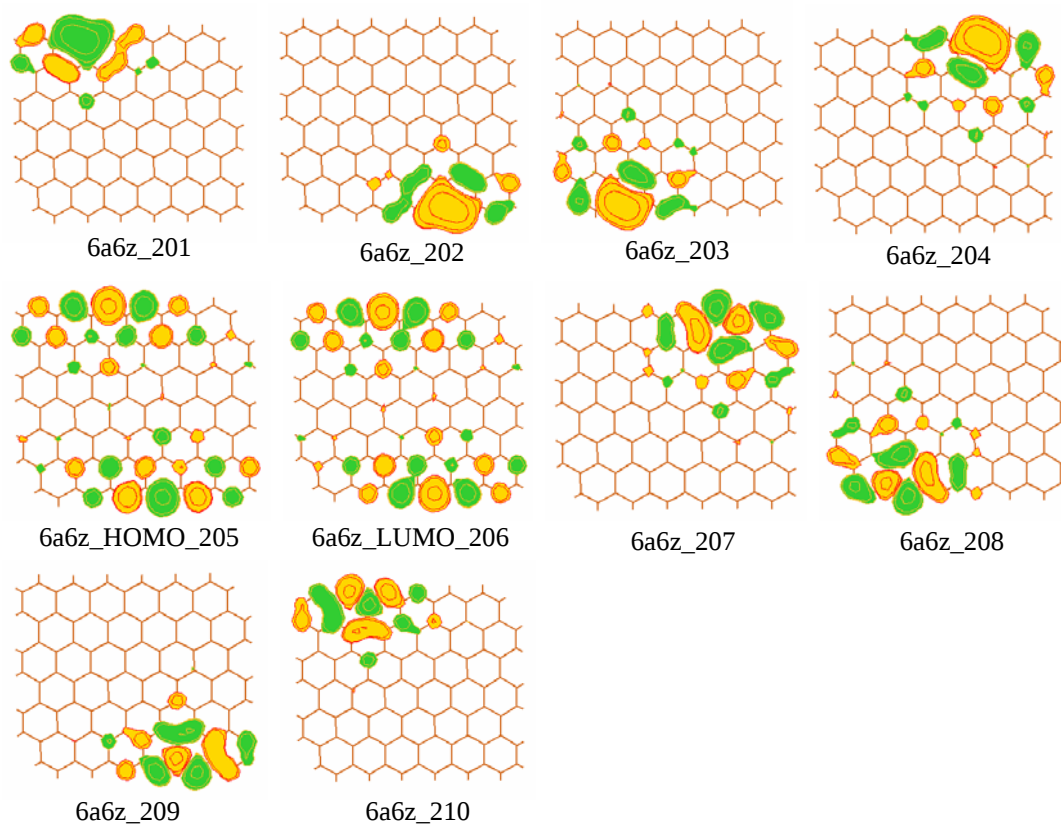
S3. The molecular orbitals of PP calculations for three systems: 4a4z with active space (12, 12), 5a5z with active space (14, 14) and 6a6z with active space (10, 10).



Singlet, Active apace (12,12)



Singlet, Active apace (14,14)



Singlet, Active space (10,10)