

## Supporting Information

# Electronic subshell splitting controls the atomic structure of charged and neutral silver clusters.

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## Structures



Total Energy -293.67226880

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.740840



Total Energy -293.96641444

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.579454



Total Energy -294.00751874

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.710248



Total Energy -440.72967470

Ag	0.000000	-0.012480	0.031109
Ag	0.000000	0.005877	-2.664722
Ag	0.000000	2.333135	-1.300769



Total Energy -440.94866441

Ag	0.000000	0.041640	0.198160
Ag	0.000000	0.062466	-2.830886
Ag	0.000000	2.222426	-1.301656



Total Energy -441.03708641

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.665838
Ag	0.000000	0.026335	-2.661235



Total Energy -587.72660844

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.687533
Ag	2.412197	0.000000	1.345303
Ag	-2.412392	-0.003964	1.345010



Total Energy -587.97277009

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.624911
Ag	2.418366	0.000000	1.312223
Ag	-2.415468	-0.001430	1.311710



Total Energy -588.03683744

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.808294
Ag	2.355419	0.000000	1.406016
Ag	-2.362717	0.017452	1.405995

Ag<sub>5</sub><sup>+</sup>

Total Energy -734.75968378

Ag	0.126320	-0.017454	-0.005146
Ag	1.350166	0.995121	2.239800
Ag	0.000897	-2.324715	-1.495157
Ag	-1.281045	1.083181	2.077980
Ag	-0.065338	-0.006233	-2.751076

Ag<sub>5</sub>

Total Energy -734.98574507

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.773980
Ag	2.392666	0.000000	1.411627
Ag	2.359525	0.000198	-1.305794
Ag	-2.324766	-0.000818	1.365675

Ag<sub>5</sub><sup>-</sup>

Total Energy -735.06418860

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.821951
Ag	2.362613	0.000000	1.544281
Ag	2.349643	-0.009000	-1.283246
Ag	-2.361073	0.018670	1.259995

Ag<sub>6</sub><sup>+</sup>

Total Energy -881.76551294

Ag	0.032126	0.092796	-0.065808
Ag	-0.406163	0.449338	2.741007
Ag	2.083661	-0.270326	1.749370
Ag	-0.652622	-2.424111	-1.171495
Ag	-0.243159	-2.055950	1.550597
Ag	1.940335	-1.922601	-0.530856

Ag<sub>6</sub>

Total Energy -882.02145828

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.690011
Ag	0.000000	0.275326	-2.682657
Ag	-2.256174	0.946930	-1.346671
Ag	-4.418141	1.674750	0.094742
Ag	-2.251665	0.839421	1.460314

Ag<sub>6</sub><sup>-</sup>

Total Energy -882.07472937

Ag	-0.000763	0.026063	0.000045
Ag	0.001375	-0.016888	2.754591

Ag	0.001374	0.077355	-2.752732
Ag	-2.370291	-0.190238	-1.378848
Ag	-4.744473	-0.454855	-0.006690
Ag	-2.370255	-0.239105	1.372089

Ag<sub>6</sub><sup>-</sup> (Planar)

TOTAL ENERGY -882.07362755

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.876202
Ag	2.351565	0.000000	1.437582
Ag	-2.007677	-1.226089	1.436592
Ag	0.744165	2.356402	1.441626
Ag	-1.868615	1.618738	1.443201

Ag<sub>7</sub><sup>+</sup>

Total Energy -1028.81308940

Ag	-0.031511	0.037347	0.045459
Ag	0.000075	-0.004463	2.797138
Ag	0.008273	0.079124	-2.708286
Ag	-0.378517	2.414593	-1.299334
Ag	-0.296893	2.386978	1.457867
Ag	0.168144	-2.362644	1.389745
Ag	0.122127	-2.318834	-1.366289

Ag<sub>7</sub>

Total Energy -1029.03127432

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.808600
Ag	2.530823	0.000000	1.228591
Ag	0.878242	2.262424	1.391356
Ag	0.871186	-2.266451	1.398185
Ag	2.276519	1.403572	3.656857
Ag	2.292566	-1.394456	3.649516

Ag<sub>7</sub><sup>-</sup>

Total Energy -1029.11321265

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.752603
Ag	2.496698	0.000000	-1.152197
Ag	2.499659	0.047485	1.598066
Ag	0.829854	-2.356743	-1.150068
Ag	3.263341	-2.309273	0.395026
Ag	0.789324	-2.377476	1.604119

Ag<sub>8</sub><sup>+</sup>

Total Energy -1175.82850683

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.747563
Ag	2.742773	0.000000	-0.882242
Ag	1.956166	-1.481190	1.393625
Ag	1.957974	1.477175	1.398568

Ag	0.542569	0.008476	-2.680719
Ag	1.186721	2.326213	-1.160869
Ag	1.183950	-2.317531	-1.172229

Ag<sub>8</sub>

Total Energy -1176.06356085

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.805095
Ag	2.478452	0.000000	1.499830
Ag	1.471115	2.354734	0.357513
Ag	-1.228098	2.080403	1.276221
Ag	-0.729559	2.344549	4.015762
Ag	1.929721	2.089950	3.172058
Ag	0.418687	4.187108	2.100801

Ag<sub>8</sub><sup>-</sup>

Total Energy -1176.12201177

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.841117
Ag	2.420853	0.000000	1.335758
Ag	1.286846	2.498899	0.534815
Ag	-1.303836	2.022723	1.439813
Ag	-0.765876	2.311019	4.221645
Ag	1.877327	2.020777	3.203312
Ag	0.206405	4.218580	2.470132

Ag<sub>9</sub><sup>+</sup>

Total Energy -1322.86944549

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.703552
Ag	2.778132	0.000000	-0.988866
Ag	2.058969	-1.425951	1.374824
Ag	4.472796	0.020381	1.115517
Ag	2.040566	1.429982	1.378613
Ag	0.604004	0.000733	-2.693589
Ag	1.149144	-2.322881	-1.145387
Ag	1.158797	2.320781	-1.151829

Ag<sub>9</sub>

Total Energy -1323.06473517

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.767155
Ag	2.473709	0.000000	1.244158
Ag	-1.744559	-1.781165	1.474752
Ag	0.981296	-2.411039	1.587007
Ag	-2.390362	-0.860869	-1.099790
Ag	0.085050	-0.861201	-2.628698
Ag	2.099680	-1.778824	-0.899721
Ag	-0.448077	-2.926869	-0.726729

Ag<sub>9</sub><sup>-</sup>

Total Energy -1323.15303735

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.773110
Ag	0.000000	0.566321	-2.990813
Ag	1.407101	2.122736	-1.162981
Ag	-1.812688	1.658953	1.516135
Ag	1.770253	1.702658	1.521934
Ag	-0.037625	3.650972	0.777084
Ag	-0.040973	2.727374	3.519028
Ag	-1.454949	2.083976	-1.165483

Ag<sub>10</sub><sup>+</sup>

Total Energy -1469.87260193

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.816031
Ag	2.816448	0.000000	-0.005087
Ag	-0.573373	-2.352681	1.404853
Ag	1.389127	-4.397295	1.400319
Ag	1.409031	2.041664	1.404832
Ag	2.809849	-0.001822	2.805742
Ag	1.400788	-2.360207	-0.595557
Ag	1.409834	-2.360740	3.396303
Ag	3.383714	-2.364413	1.398769

Ag<sub>10</sub>

TE -1470.08855166

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.762240
Ag	2.515981	0.000000	1.382172
Ag	1.485306	2.328782	-0.010513
Ag	-1.274423	2.448691	-0.574147
Ag	-2.313077	0.820301	1.392537
Ag	1.499284	2.322019	2.748962
Ag	-0.216381	4.088608	1.377944
Ag	-1.253099	2.450941	3.345347
Ag	-3.035932	3.608134	1.389795

Ag<sub>10</sub><sup>-</sup>

Total Energy -1470.16842438

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.849254
Ag	2.461993	0.000000	1.421880
Ag	2.172419	1.797295	3.506497
Ag	-1.653761	1.805922	1.279564
Ag	-0.502316	2.580011	3.703207
Ag	-0.913752	4.495078	1.661491
Ag	1.486409	4.485763	3.036212
Ag	1.064549	2.461085	1.010437
Ag	0.842161	-2.276570	1.381019

Ag<sub>11</sub><sup>+</sup>

Total Energy -1616.89996212

Ag	-0.464727	1.604071	-0.411832
Ag	-2.401439	-0.116408	0.427431
Ag	2.184219	0.326820	0.332680
Ag	-0.070795	0.275671	2.075695
Ag	0.053037	-1.154651	-0.479888
Ag	-1.234877	-2.232004	2.072002
Ag	1.572847	-1.971766	2.165030
Ag	-2.052691	-2.888094	-0.591105
Ag	0.389272	-3.859043	0.353864
Ag	2.840753	-4.441493	1.433218
Ag	2.628901	-2.365801	-0.412296

Ag<sub>11</sub>

Total Energy -1617.10524542

Ag	-0.550177	0.181485	-0.052631
Ag	-0.493476	0.301164	2.763594
Ag	2.433678	0.023739	-0.245343
Ag	1.853161	1.624714	3.887028
Ag	1.716224	-1.132473	4.008465
Ag	3.836010	1.429259	1.827013
Ag	0.988666	-1.642442	1.398393
Ag	3.703782	-1.336185	1.938131
Ag	4.200540	0.129481	4.394947
Ag	1.170523	1.962512	1.242964
Ag	6.148169	-0.035454	2.482938

Ag<sub>11</sub><sup>-</sup>

Total Energy -1617.20160464

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.931574
Ag	0.000000	1.315302	-2.554733
Ag	-2.045943	1.531270	4.036760
Ag	-2.348875	0.267286	1.449183
Ag	2.444338	0.585245	-1.270009
Ag	0.858050	2.872704	-0.467800
Ag	2.074408	1.215042	1.419995
Ag	-3.312019	2.808286	1.821408
Ag	-1.851253	2.160949	-0.550601
Ag	-0.457067	2.578978	1.957126

Ag<sub>12</sub><sup>+</sup>

Total Energy -1763.92126824

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.871303
Ag	2.643264	0.000000	-0.986584
Ag	1.193195	-2.346035	3.839427
Ag	1.799280	-3.966030	1.589326
Ag	-0.172804	-4.573574	-0.415491
Ag	0.177085	-3.534078	-3.132363
Ag	0.521909	-0.771700	-2.835865

Ag	-1.349795	-2.124900	-1.207710
Ag	-0.490677	-2.380537	1.460308
Ag	1.534564	-2.503372	-0.882105
Ag	2.166297	-1.131024	1.527572

Ag<sub>12</sub>

Total Energy -1764.13255873

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.820808
Ag	2.422253	0.000000	1.250638
Ag	0.944757	2.309653	1.683649
Ag	-1.753514	1.792067	1.330760
Ag	-0.287274	3.681356	-0.340892
Ag	-1.655033	1.601098	-1.563060
Ag	0.364346	3.066543	-3.093625
Ag	0.452512	0.314414	-2.764765
Ag	2.763125	1.546722	-3.611202
Ag	1.959811	2.121984	-0.943932
Ag	2.829123	-0.401207	-1.522266

Ag<sub>12</sub><sup>-</sup>

Total Energy -1764.21559993

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.772457
Ag	2.672671	0.000000	-0.884287
Ag	3.468235	1.427911	-3.127730
Ag	-1.513184	2.270239	-0.693999
Ag	-2.421263	0.630796	1.362317
Ag	-0.561032	2.634792	1.913204
Ag	1.975275	1.499069	1.413395
Ag	3.547562	2.643477	-0.619553
Ag	2.174779	3.933504	-2.752807
Ag	0.769230	1.606757	-2.214820
Ag	0.929871	3.650723	-0.239748

Ag<sub>13</sub><sup>+</sup>

Total Energy -1910.94552516

Ag	-0.074138	1.308374	-0.124729
Ag	-0.562913	-0.659022	1.872974
Ag	1.923886	-0.671833	0.358606
Ag	1.365330	-2.817029	2.242162
Ag	2.693670	-3.255449	-0.118123
Ag	2.254390	1.376427	-1.536702
Ag	-0.117977	1.971792	-2.882507
Ag	-2.480605	1.946939	-1.458173
Ag	-2.399774	1.403622	1.283629
Ag	-1.342270	-3.244713	2.343975
Ag	-0.093130	-2.688190	-0.153701
Ag	0.344712	-0.749825	-2.078462
Ag	-2.032740	-0.762408	-0.609963



Ag<sub>13</sub>  
Total Energy -1911.14498060  
Ag 0.000000 0.000000 0.000000  
Ag 0.000000 0.000000 2.756823  
Ag 1.325507 0.000000 -2.408626  
Ag 3.177764 -1.607805 -1.064474  
Ag 2.262710 -3.719560 0.467840  
Ag -0.057018 -2.500162 1.393369  
Ag 0.559730 -2.497257 -1.413105  
Ag 2.286346 1.602563 2.510896  
Ag 2.236461 3.712431 0.716626  
Ag 2.370733 -1.110434 1.588136  
Ag 2.828515 1.096451 -0.208872  
Ag -0.158660 2.491713 1.509560  
Ag 0.649659 2.512518 -1.241281

Ag<sub>13</sub><sup>-</sup>  
Total Energy -1911.24815663  
Ag 0.000000 0.000000 0.000000  
Ag 0.000000 0.000000 2.725149  
Ag 2.422731 0.000000 1.249453  
Ag 0.290834 -0.028672 5.409531  
Ag 4.678267 -0.025082 2.728255  
Ag 6.967672 -0.116928 4.272084  
Ag 0.631330 0.015815 8.153662  
Ag 2.346525 1.361945 3.827939  
Ag 2.272451 1.691539 6.620876  
Ag 4.637015 0.964535 5.443839  
Ag 2.319309 -1.409750 3.807651  
Ag 4.837725 -1.780399 5.009706  
Ag 2.720149 -1.059144 6.589505

Ag<sub>14</sub><sup>+</sup>  
Total Energy -2057.97625288  
Ag 0.000000 0.000000 0.000000  
Ag 0.000000 0.000000 2.822819  
Ag 2.428723 0.000000 1.366514  
Ag 3.834723 2.207982 2.377307  
Ag 1.054053 2.421380 1.863935  
Ag -1.657646 1.795050 1.398891  
Ag 4.843820 0.792761 0.145830  
Ag 4.586204 1.899232 -2.374834  
Ag 2.453223 0.248759 -1.450026  
Ag -0.047632 0.674631 -2.757017  
Ag -2.312290 1.207059 -1.223437  
Ag 0.065714 2.716302 -0.770250  
Ag 1.956478 2.648122 -2.908224  
Ag 2.871345 2.763859 -0.218855

Ag<sub>14</sub>  
Total Energy -2057.97160095

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.845810
Ag	2.402583	0.000000	1.402633
Ag	3.799875	2.410156	1.279237
Ag	2.208186	1.636328	-0.928484
Ag	-2.541120	0.688627	3.865720
Ag	-2.424668	-0.636461	1.372427
Ag	-0.352562	2.463961	4.035273
Ag	1.045069	2.589592	1.544890
Ag	2.308429	1.536145	3.768177
Ag	-2.418597	0.822837	-1.056152
Ag	0.147004	0.754206	-2.662417
Ag	-0.400243	2.779813	-0.828369
Ag	-1.747595	2.036601	1.516709

Ag<sub>14</sub><sup>-</sup>

Total Energy -2058.26467339

Ag	0.00000	0.00000	0.00000
Ag	0.00000	0.00000	2.80151
Ag	0.94903	0.00000	-2.62023
Ag	0.72376	2.28702	1.45070
Ag	3.42813	2.75241	1.85838
Ag	2.08517	-1.44096	3.96653
Ag	0.17571	-2.45442	-1.31448
Ag	2.65017	-1.26255	-0.80978
Ag	2.83055	-0.01265	1.69471
Ag	2.66350	1.48095	-0.67339
Ag	0.17560	2.43077	-1.43985
Ag	1.08571	-2.26264	1.39727
Ag	2.08501	1.45095	3.95133
Ag	2.03330	4.19505	-0.17737

Ag<sub>15</sub><sup>+</sup>

Total Energy -2205.0168005

Ag	0.00000	0.00000	0.00000
Ag	0.00000	0.00000	2.76795
Ag	2.55442	0.00000	-1.26901
Ag	0.89470	2.29639	-1.36999
Ag	2.84836	2.02175	-3.31200
Ag	1.70696	1.83790	1.32359
Ag	2.36967	-0.88379	1.39014
Ag	4.88921	-0.48624	0.21651
Ag	2.49238	0.60839	3.80552
Ag	4.42808	1.63875	1.98299
Ag	3.66692	2.47696	-0.58555
Ag	5.11526	0.76714	-2.33396
Ag	4.68883	-0.98190	3.04579
Ag	6.41293	1.88627	-0.09596
Ag	6.96267	0.26948	2.08218

Ag<sub>15</sub>  
Total Energy -2205.21103635

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.903482
Ag	0.000000	1.113984	-2.721359
Ag	-2.273318	1.537065	3.861586
Ag	-3.407058	2.887735	1.606352
Ag	-1.522581	3.537079	-2.740763
Ag	2.380685	0.691504	-1.325156
Ag	1.994896	1.379900	1.398122
Ag	-2.431700	0.178314	1.431443
Ag	-4.710986	1.077422	-0.058822
Ag	-4.026988	3.631058	-1.197087
Ag	-1.616121	4.350938	0.014657
Ag	-0.611072	2.470828	1.805897
Ag	0.635921	2.830248	-0.663166
Ag	-2.118754	1.608321	-0.895581

Ag<sub>15</sub><sup>-</sup>  
Total Energy -2205.30684300

Ag	0.000000	0.000000	0.000000
Ag	0.000000	0.000000	2.803627
Ag	2.448933	0.000000	-1.356632
Ag	-0.856394	2.499730	3.780408
Ag	1.789183	2.375044	-0.007950
Ag	1.777237	2.369674	2.797870
Ag	2.476218	0.000737	1.455120
Ag	0.375792	1.569857	-2.389416
Ag	-1.772288	3.173872	-3.141399
Ag	-2.226843	0.979984	-1.444555
Ag	0.213991	4.232464	-1.452567
Ag	-2.759859	3.934844	2.289086
Ag	-2.352139	3.622785	-0.459762
Ag	-0.123075	3.817487	1.336101
Ag	-1.922075	1.428224	1.342268