Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Quintuple super bonding between superatoms of metallic clusters

by

Haiyan Wang[a], and Longjiu Cheng[a,b]*

[a]Department of Chemistry, Anhui University, Hefei, Anhui, 230601, PR China.

Email: clj@ustc.edu.

[b]AnHui Province Key Laboratory of Chemistry for Inorganic/Organic Hybrid Functionalized Materials, Hefei, Anhui 230601, P. R. China..

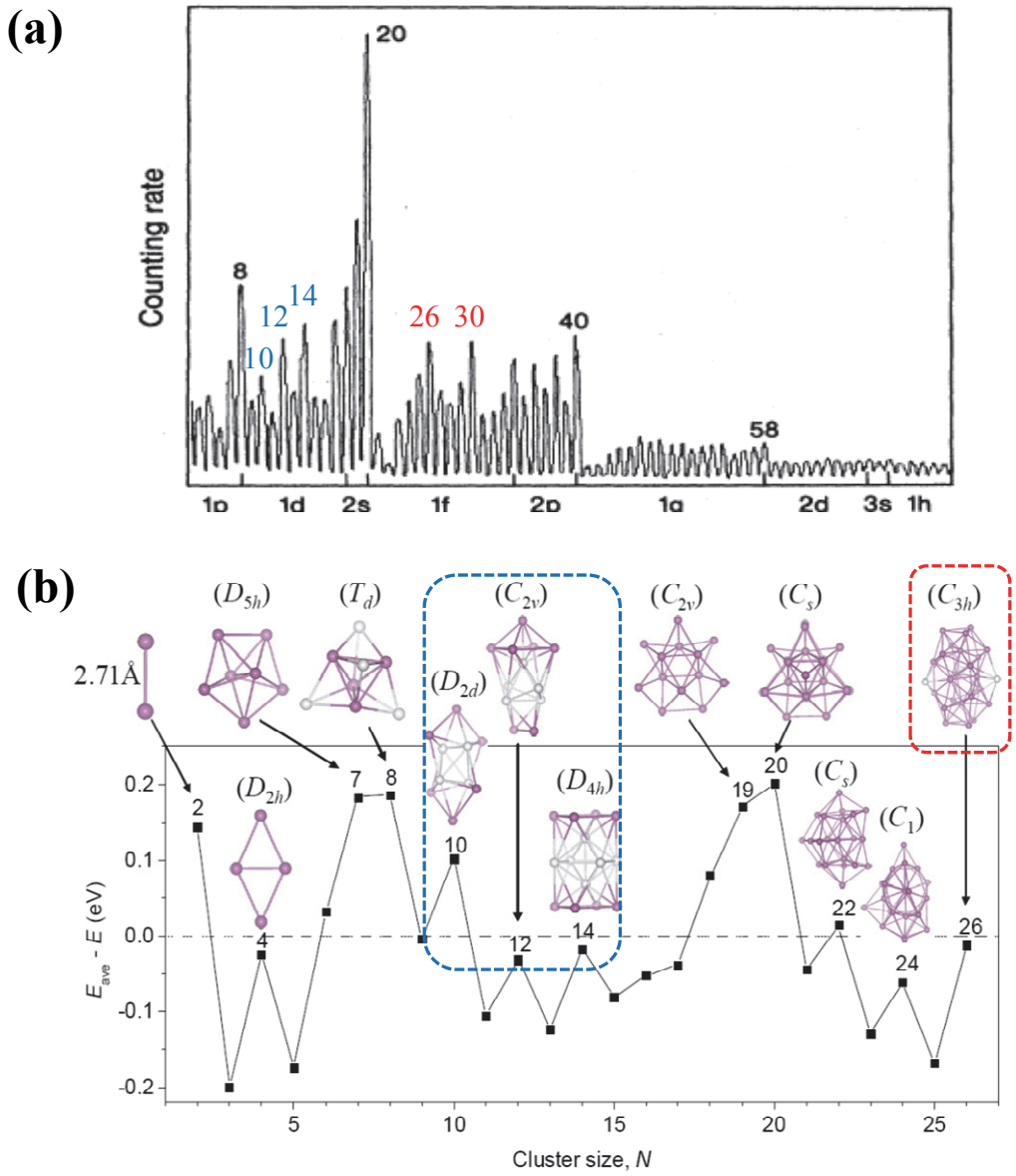

Figure S1. (a) Mass spectra of sodium clusters (Phys. Rev. Lett. 1984, 52, 2141). (b) Relative stability of lithium clusters calculated at B3LYP/6-311+G* level of theory (J. Chem. Phys. 2013, 138, 141101), where positive peaks represent higher stability.

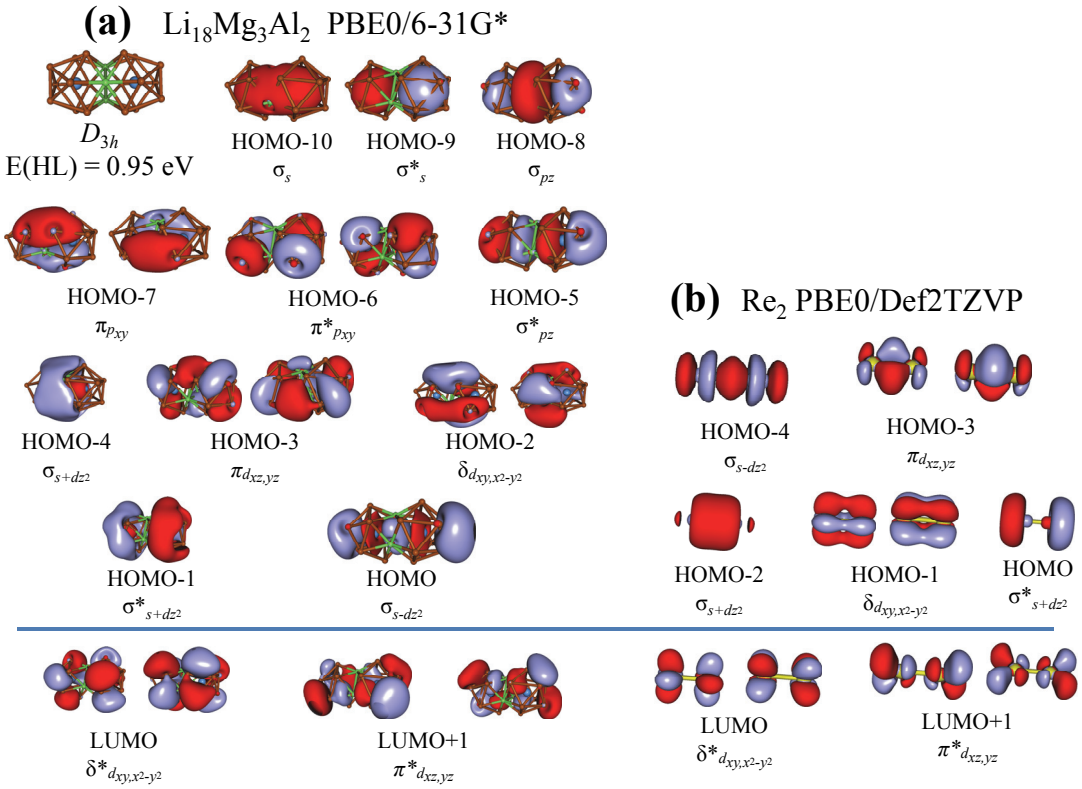

Figure S2. Canonical molecular orbital diagrams of a) $Li_{18}Mg_3Al_2$ cluster (PBE0/6-31G*) and (b) Re_2 molecule (PBE0/def2-TZVP)..

XYZ coordinates (Å) of the structures discussed in this paper.
Li26 clusters

A1

Li	-1.350380	1.531166	-4.563591
Li	0.426943	3.033581	-2.438428
Li	1.717956	1.006505	-4.585830
Li	-2.235808	1.937201	-1.384455
Li	-0.270603	-1.379113	-4.797819
Li	-2.256925	1.684789	1.654105
Li	0.017848	0.213430	-2.569240
Li	-0.835925	4.223498	0.345023
Li	0.182834	1.639741	0.137480
Li	2.706387	1.158595	-1.414798
Li	-2.666014	-1.274043	2.569047
Li	2.257634	-1.537343	-2.805391
Li	-1.516403	-0.661195	-0.065465
Li	-0.438854	-2.717251	-1.758583
Li	-1.415013	0.758779	4.734589
Li	0.389757	2.589204	2.911184
Li	1.333501	-0.978423	-0.072008
Li	-0.017857	-0.213407	2.569239
Li	-2.628837	-0.829655	-2.780600
Li	2.685266	0.906187	1.623798
Li	-0.335213	-2.151493	4.500323
Li	-3.251743	-2.831089	-0.257775
Li	4.087620	-1.392433	-0.087259
Li	-0.459969	-2.969651	1.279939
Li	2.220452	-1.981724	2.544202
Li	1.653345	0.234143	4.712314

A2

Li	1.698022	-0.916287	4.747866
Li	2.486036	1.395254	2.720314
Li	2.821483	-1.503590	1.564459
Li	-0.061394	1.665866	4.604388
Li	0.474079	-3.136689	2.789005
Li	0.186530	-0.305938	2.578133
Li	-1.373501	-1.192198	4.677577
Li	2.670800	3.234497	0.000000
Li	2.821483	-1.503590	-1.564459
Li	1.573848	0.601863	0.000000
Li	0.410985	-1.990202	0.000000
Li	0.010260	2.533969	1.511225
Li	-2.407346	0.963545	2.625023
Li	0.474079	-3.136689	-2.789005
Li	2.486036	1.395254	-2.720314
Li	-2.704148	2.851244	0.000000
Li	1.698022	-0.916287	-4.747866
Li	-2.105418	-1.989412	1.549750
Li	-4.071058	-0.071427	0.000000
Li	0.186530	-0.305938	-2.578133
Li	-1.337928	0.344983	0.000000
Li	-2.105418	-1.989412	-1.549750
Li	0.010260	2.533969	-1.511225
Li	-1.373501	-1.192198	-4.677577
Li	-0.061394	1.665866	-4.604388
Li	-2.407346	0.963545	-2.625023

A3

Li	0.484132	1.775011	4.705497
Li	-1.921640	2.089492	2.727534
Li	-1.667827	-0.476340	4.639372
Li	0.775486	2.909200	1.553396
Li	1.319232	-1.231286	4.651518
Li	0.775486	2.909200	-1.553396
Li	0.075078	0.066734	2.577955
Li	-3.599618	2.154585	0.000000
Li	-1.031006	1.264879	0.000000
Li	-2.684428	-0.663540	1.492757

Li	2.796158	0.843377	-2.705109
Li	-0.649251	-2.714641	2.663332
Li	1.644054	0.496888	0.000000
Li	2.153353	-1.941151	1.525516
Li	0.484132	1.775011	-4.705497
Li	-1.921640	2.089492	-2.727534
Li	-0.351925	-1.566185	0.000000
Li	0.075078	0.066734	-2.577955
Li	2.796158	0.843377	2.705109
Li	-2.684428	-0.663540	-1.492757
Li	1.319232	-1.231286	-4.651518
Li	4.322162	-0.133767	0.000000
Li	-2.344253	-3.530114	0.000000
Li	2.153353	-1.941151	-1.525516
Li	-0.649251	-2.714641	-2.663332
Li	-1.667827	-0.476340	-4.639372

A4

Li	-1.126333	1.126333	1.126333
Li	1.126333	-1.126333	1.126333
Li	1.126333	1.126333	-1.126333
Li	1.779410	1.779410	1.779410
Li	0.000000	0.000000	3.569644
Li	-1.779410	-1.779410	1.779410
Li	-1.126333	-1.126333	-1.126333
Li	-1.779410	1.779410	-1.779410
Li	0.000000	3.569644	0.000000
Li	-3.569644	0.000000	0.000000
Li	-3.078257	0.840340	3.078257
Li	-0.840340	3.078257	3.078257
Li	-3.078257	3.078257	0.840340
Li	1.779410	-1.779410	-1.779410
Li	0.000000	-3.569644	0.000000
Li	3.569644	0.000000	0.000000
Li	3.078257	-0.840340	3.078257
Li	0.840340	-3.078257	3.078257
Li	3.078257	-3.078257	0.840340
Li	0.000000	0.000000	-3.569644
Li	3.078257	0.840340	-3.078257
Li	0.840340	3.078257	-3.078257
Li	3.078257	3.078257	-0.840340
Li	-3.078257	-3.078257	-0.840340
Li	-3.078257	-0.840340	-3.078257
Li	-0.840340	-3.078257	-3.078257

A5

Li	-2.742638	1.583483	1.877091
Li	-0.000016	1.952005	0.871339
Li	-2.684013	-1.549674	3.448533
Li	-1.690662	-0.976152	0.871508
Li	-1.545921	0.892539	4.956193
Li	-0.000079	3.099255	3.448339
Li	1.690326	-0.975893	0.871357
Li	-0.000072	-0.000145	2.873021
Li	2.742467	1.583569	1.877076
Li	0.000048	-1.785167	4.956350
Li	-0.000207	-3.166778	1.877185
Li	2.683984	-1.549724	3.448313
Li	1.546000	0.892491	4.956130
Li	-1.546000	-0.892491	-4.956130
Li	-2.683984	1.549724	-3.448313
Li	-0.000048	1.785167	-4.956350
Li	-2.742467	-1.583569	-1.877076
Li	1.545921	-0.892539	-4.956193
Li	0.000072	0.000145	-2.873021
Li	-1.690326	0.975893	-0.871357
Li	0.000207	3.166778	-1.877185
Li	2.684013	1.549674	-3.448533
Li	0.000016	-1.952005	-0.871339

Li	2.742638	-1.583483	-1.877091
Li	1.690662	0.976152	-0.871508
Li	0.000079	-3.099255	-3.448339

Li20Mg3 clusters

B1

Li	-4.617647	-0.004062	1.808923
Li	-4.617613	-1.564559	-0.908027
Li	-4.617613	1.568622	-0.900991
Li	-2.740628	0.006585	-2.932755
Li	-2.496355	0.000000	-0.000025
Li	1.554381	-2.508719	-1.455887
Li	4.617614	-1.564559	-0.908027
Li	2.496356	-0.000000	-0.000025
Li	4.617614	1.568621	-0.900991
Li	4.617647	-0.004062	1.808923
Li	2.740665	-2.543134	1.460670
Li	-1.554380	-2.508720	-1.455887
Li	-2.740665	-2.543134	1.460670
Li	-1.554424	-0.006513	2.900583
Li	1.554425	-0.006513	2.900582
Li	-1.554380	2.515233	-1.444606
Li	-2.740664	2.536549	1.472077
Li	2.740665	2.536549	1.472076
Li	1.554381	2.515233	-1.444605
Li	2.740628	0.006586	-2.932755
Mg	-0.000000	0.004024	-1.791871
Mg	-0.000000	-1.553841	0.892461
Mg	-0.000000	1.549817	0.899430

B2

Li	1.627265	4.358830	0.000000
Li	0.010000	3.197936	2.505477
Li	-1.599906	4.368981	0.000001
Li	-2.774567	-1.590286	2.505471
Li	0.009998	3.197937	-2.505477
Li	-4.588528	-0.770070	-0.000001
Li	-2.510882	1.460171	1.483188
Li	-0.000028	0.000065	2.307833
Li	-2.510883	1.460170	-1.483188
Li	2.519963	1.444482	1.483198
Li	-2.774566	-1.590288	-2.505471
Li	-0.000028	0.000065	-2.307833
Li	2.764555	-1.607659	2.505492
Li	-0.009151	-2.904504	1.483221
Li	2.519962	1.444483	-1.483198
Li	-2.983826	-3.570029	0.000001
Li	2.961279	-3.588686	-0.000000
Li	4.583637	-0.798912	0.000000
Li	-0.009150	-2.904504	-1.483221
Li	2.764555	-1.607658	-2.505492
Mg	0.005914	1.878562	-0.000000
Mg	-1.629906	-0.934234	-0.000000
Mg	1.624068	-0.944459	-0.000000

B3

Li	-1.483125	-4.517645	0.000000
Li	1.333498	-4.303224	1.569869
Li	1.333498	-4.303224	-1.569869
Li	3.284063	-1.830710	0.000000
Li	1.594975	1.691314	2.482438
Li	1.372935	4.711677	1.538143
Li	0.177410	2.720739	0.000000
Li	1.372935	4.711677	-1.538143
Li	-1.436722	4.935204	0.000000
Li	-1.219793	3.075340	2.487754
Li	1.574421	-1.241551	2.517728
Li	-1.292262	-2.575185	2.561167

Li	-2.802279	-1.397910	0.000000
Li	-2.750421	1.884285	0.000000
Li	1.574421	-1.241551	-2.517728
Li	-1.292262	-2.575185	-2.561167
Li	-1.219793	3.075340	-2.487754
Li	1.594975	1.691314	-2.482438
Li	3.287127	2.352915	0.000000
Li	1.573213	0.253562	0.000000
Mg	-0.899986	0.229623	1.613232
Mg	-0.899986	0.229623	-1.613232
Mg	0.155768	-2.238541	0.000000

B4

Li	1.660680	4.615211	0.592780
Li	-1.660680	4.615211	0.592780
Li	-0.000000	4.525658	-2.129363
Li	-2.643098	2.364616	-1.688660
Li	-2.535315	-1.523274	1.301176
Li	-1.660680	-4.615211	0.592780
Li	-0.000000	-4.525658	-2.129363
Li	1.660680	-4.615211	0.592780
Li	0.000000	-2.853245	2.726497
Li	-2.535315	1.523274	1.301176
Li	0.000000	2.853245	2.726497
Li	2.535315	1.523274	1.301176
Li	2.535315	-1.523274	1.301176
Li	-0.000000	1.429719	-3.055911
Li	2.643098	2.364616	-1.688660
Li	2.643098	-2.364616	-1.688660
Li	-0.000000	-1.429719	-3.055911
Li	-2.643098	-2.364616	-1.688660
Li	-1.428730	0.000000	-0.911181
Li	1.428730	-0.000000	-0.911181
Mg	0.000000	2.442105	-0.177614
Mg	0.000000	-0.000000	1.834911
Mg	-0.000000	-2.442105	-0.177614

Li18Mg3Al2 clusters

C1

Mg	0.000000	1.785947	0.000000
Mg	-1.546675	-0.892973	0.000000
Mg	1.546675	-0.892973	0.000000
Al	0.000000	0.000000	2.620490
Al	0.000000	0.000000	-2.620490
Li	0.000000	-1.714784	4.753163
Li	-1.485047	0.857392	4.753163
Li	1.485047	0.857392	4.753163
Li	0.000000	2.848454	2.809608
Li	-2.466833	-1.424227	2.809608
Li	2.466833	-1.424227	2.809608
Li	-2.439155	1.408247	1.592569
Li	2.439155	1.408247	1.592569
Li	0.000000	-2.816494	1.592569
Li	-2.439155	1.408247	-1.592569
Li	2.439155	1.408247	-1.592569
Li	0.000000	-2.816494	-1.592569
Li	-2.466833	-1.424227	-2.809608
Li	2.466833	-1.424227	-2.809608
Li	0.000000	2.848454	-2.809608
Li	0.000000	-1.714784	-4.753163
Li	1.485047	0.857392	-4.753163
Li	-1.485047	0.857392	-4.753163