Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

On the energetic and magnetic stability of neutral and charged lithium clusters doped with one and two yttrium atoms

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Supplementary information

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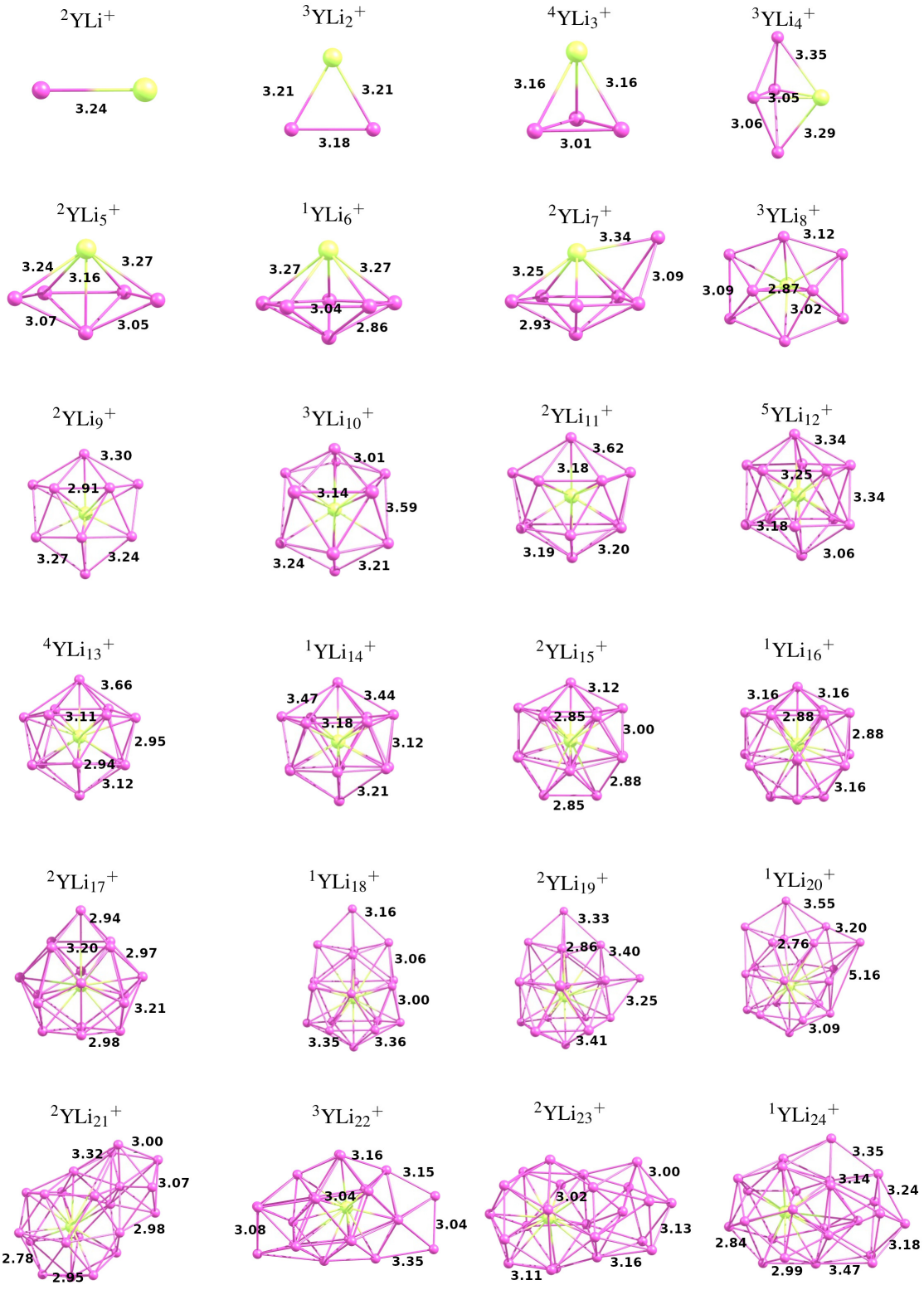

Fig. S1 Ground-state geometries of YLi_n^+ clusters for $n = 1-24$. The superscripts indicate spin multiplicity. Selected bond lengths are given in angstroms.

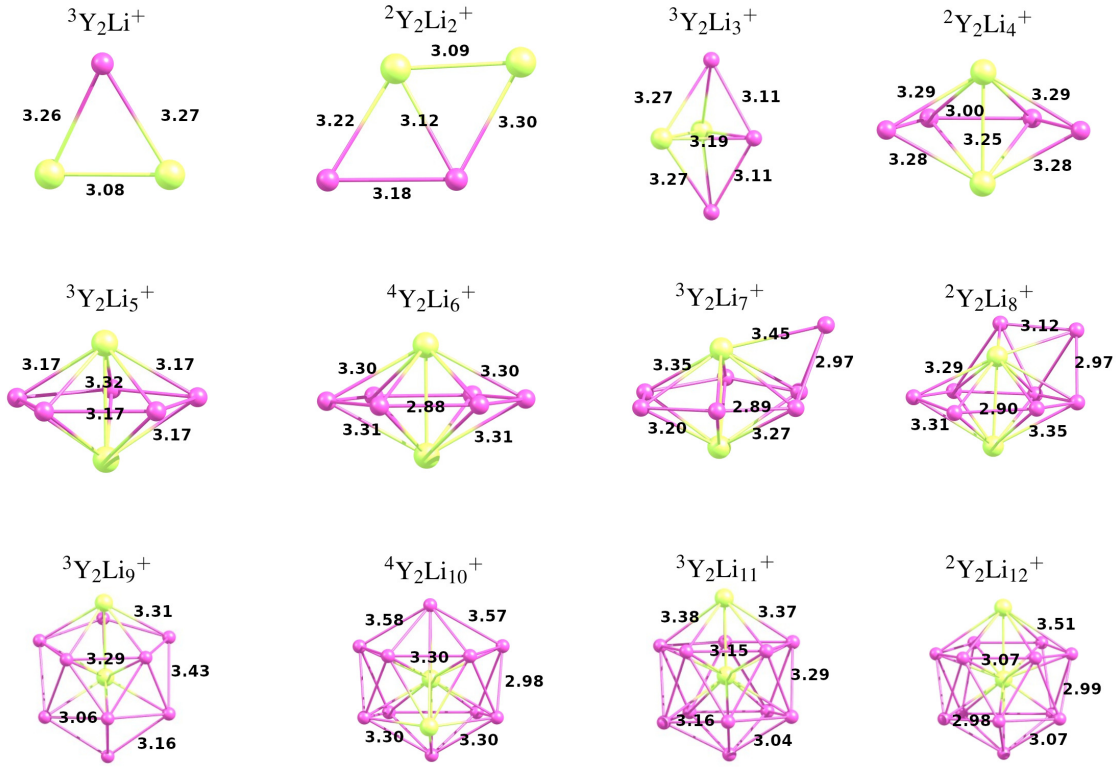

Fig. S2 Ground-state geometries of $Y_2Li_n^+$ clusters for $n = 1 - 12$. The superscripts indicate spin multiplicity. Selected bond lengths are given in angstroms.

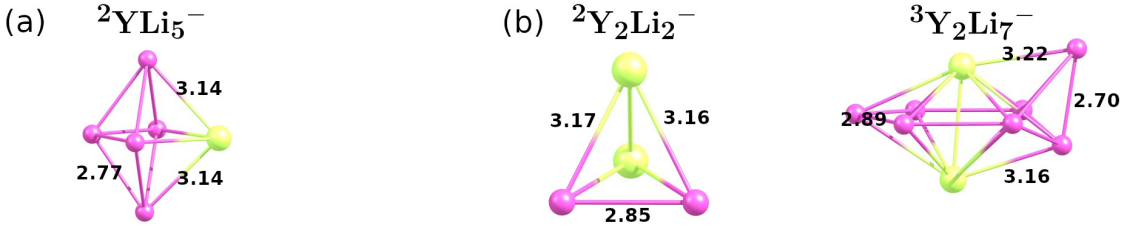

Fig. S3 Ground state geometries for (a) the YLi_5^- anion cluster, whose geometry is similar to the neutral case, but different from the cation, and (b) the $Y_2Li_2^-$ and $Y_2Li_7^-$ anion clusters, whose geometries are similar to the neutral case, but different from the cation. The superscripts indicate spin multiplicity. Selected bond lengths are given in angstroms.

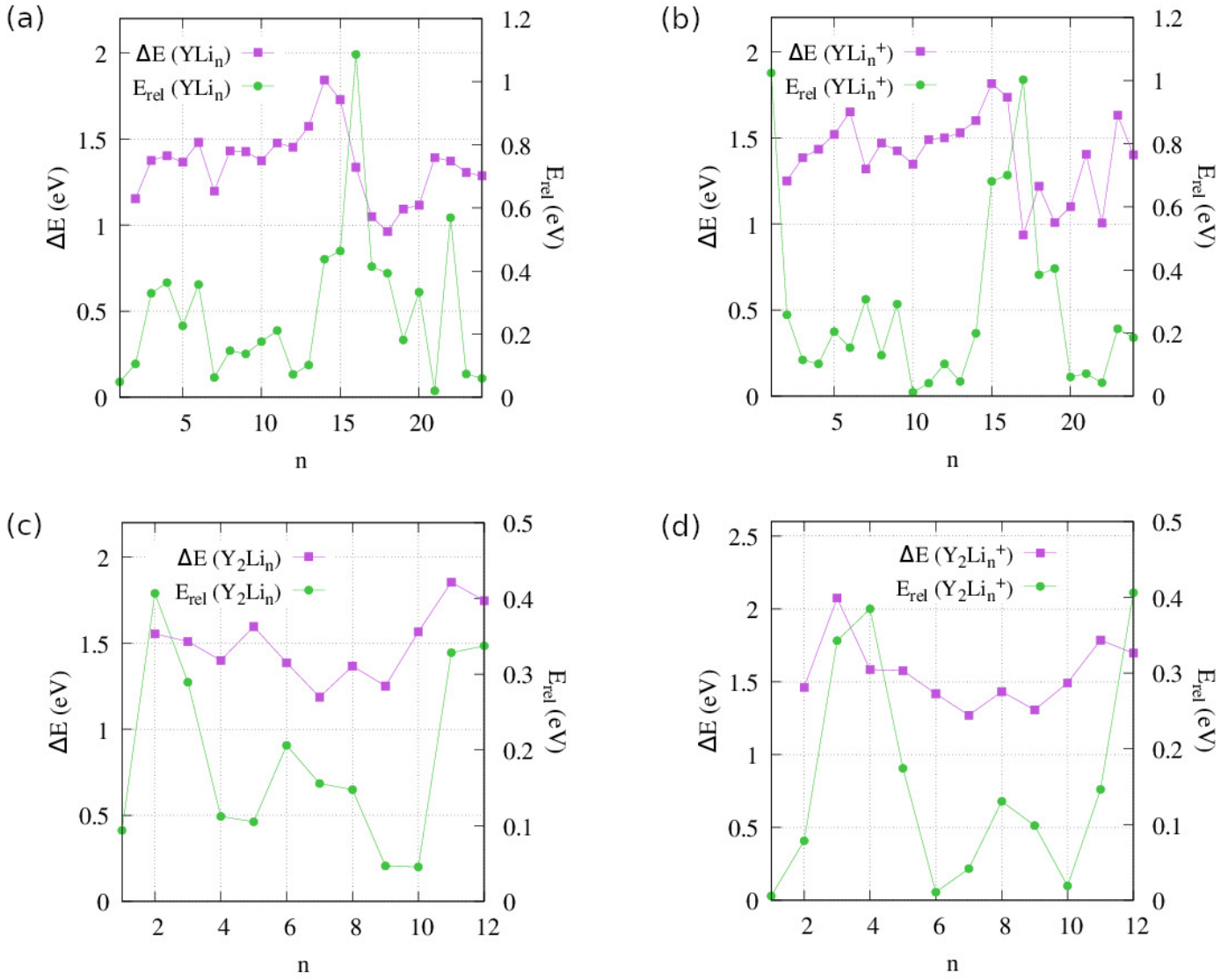

Fig. S4 Variation in the energy gain ΔE and relative energy to the lowest isomer of different spin multiplicity (E_{rel}) with the number of alkali Li atoms in: (a) the YLi_n ($n = 1-24$) clusters, (b) the YLi_n^+ ($n = 1-24$) clusters, (c) the Y_2Li_n ($n = 1-12$) clusters, and (d) the $Y_2Li_n^+$ ($n = 1-12$) clusters. Units are in eV.

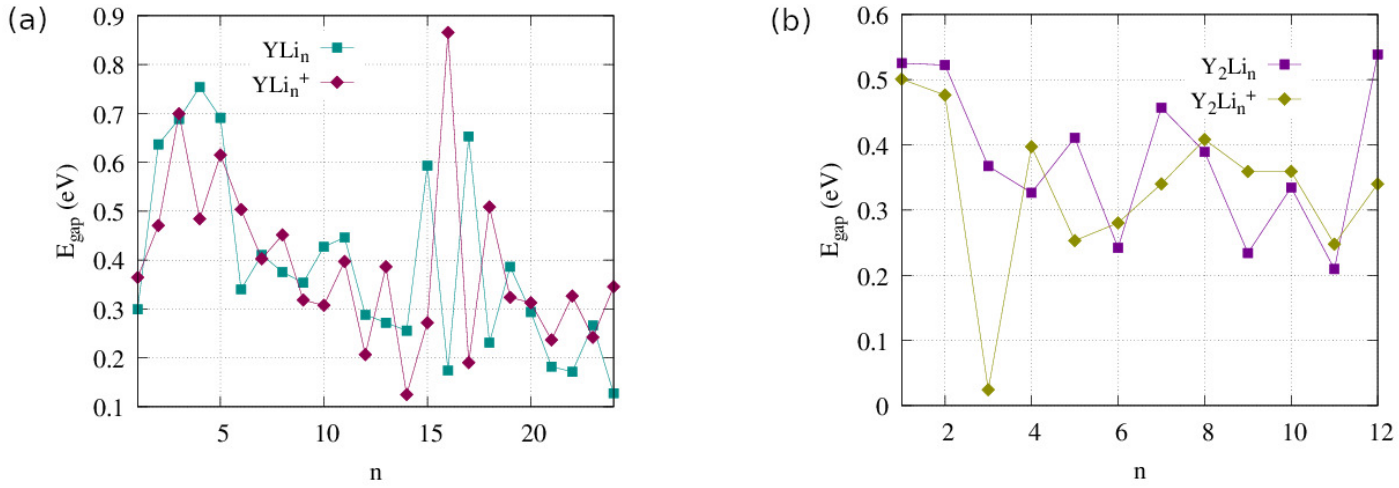

Fig. S5 Variation in the the energy gap: (a) in the YLi_n clusters and YLi_n^+ clusters, for $n = 1-24$, (b) in the Y_2Li_n clusters, and in the $Y_2Li_n^+$ clusters, for $n = 1-12$. Units are in eV.

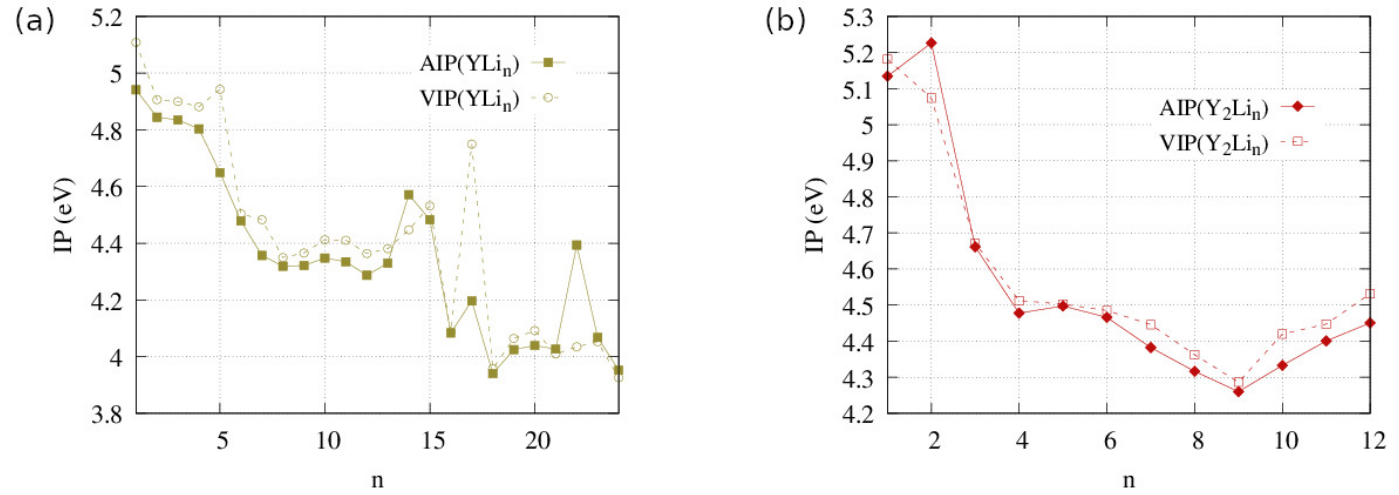

Fig. S6 Adiabatic ionization energies (AIP) and vertical ionization energies (VIP): (a) in YLi_n clusters ($n = 1-24$), (b) in Y_2Li_n clusters ($n = 1-12$). Units are in eV.

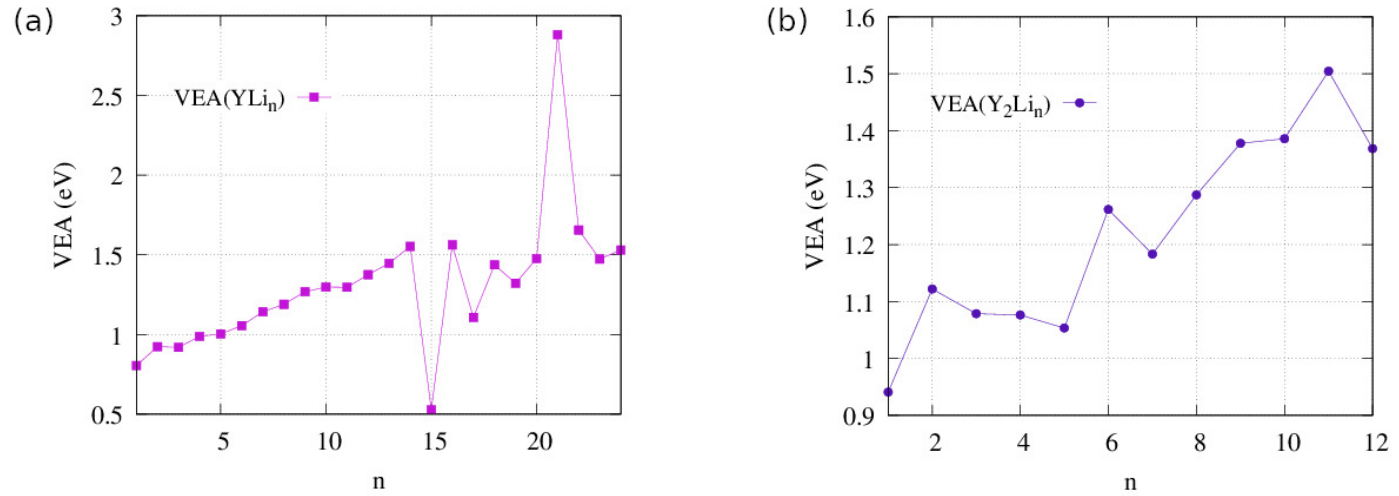

Fig. S7 Vertical electron affinity (VEA): (a) in YLi_n clusters, (b) in Y_2Li_n clusters. Units are in eV.

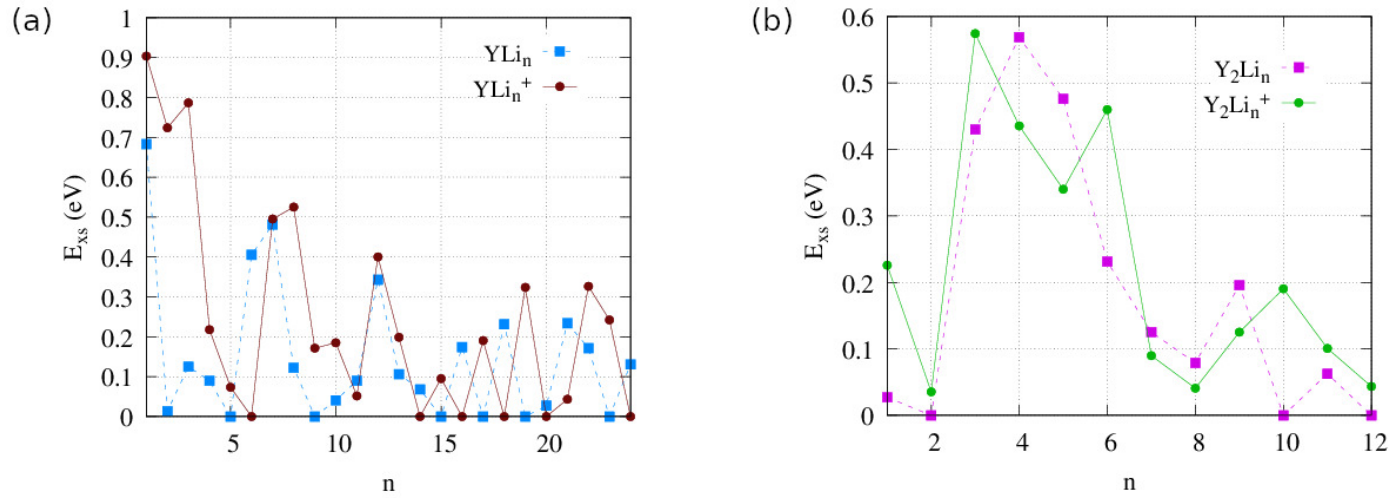

Fig. S8 Exchange-splitting: (a) in the YLi_n and YLi_n^+ clusters for $n = 1-24$, (b) in the Y_2Li_n and $Y_2Li_n{}^+$ clusters. Units are in eV.

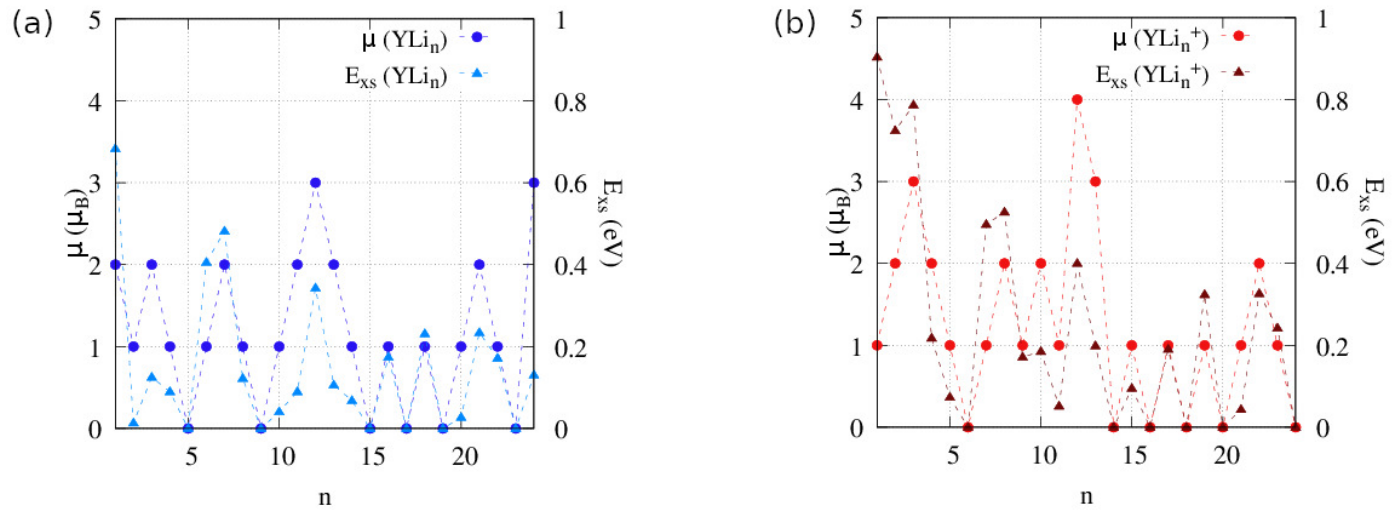

Fig. S9 Correlation between exchange-splitting and magnetic moment for the clusters : (a) YLi_n $(n = 1-24)$, (b) $YLi_n{}^+$ $(n = 1-24)$. The units of E_{xs} are in eV and for μ in μ_B.

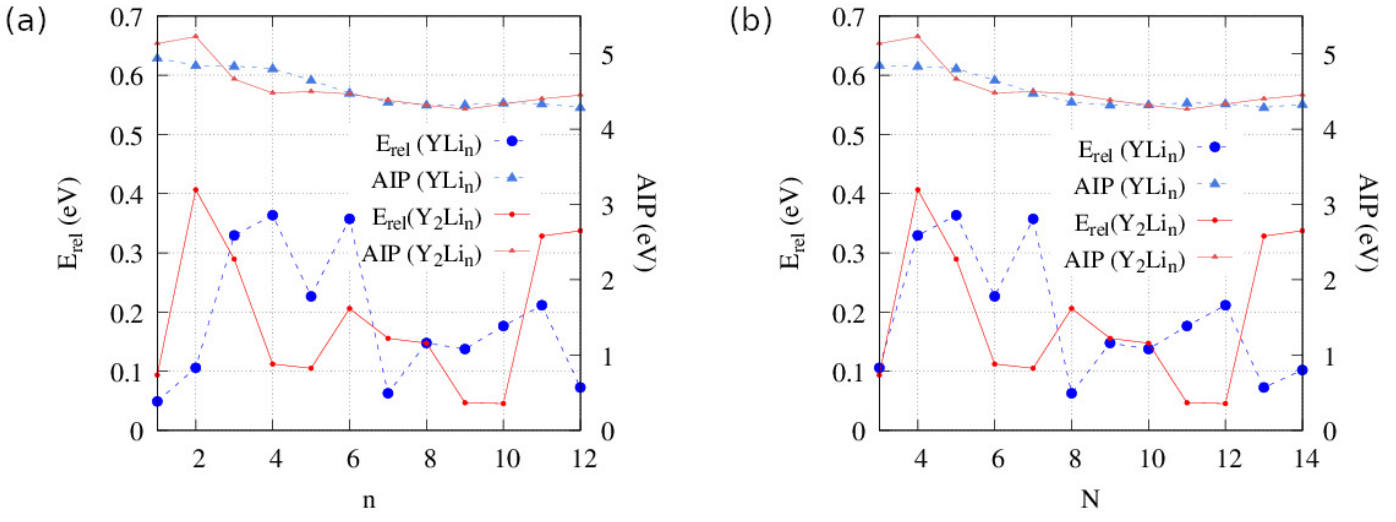

Fig. S10 Correlation in the E_{rel} values and AIP values for the YLi_n and Y_2Li_n clusters, in terms of: (a) the increase in the number n of lithium atoms, (b) the increase of the number $N = 3-14$ of atoms. Units are in eV.

Table S1 Atomization energy (AE), energy gain (ΔE), exchange splitting E_{xs}, energy gap (E_{gap}) and magnetic moment (μ), for the charged YLi_n^+ ($n = 1-24$) clusters and charged $Y_2Li_n^+$ ($n = 1-12$) clusters. The magnetic moment (μ) and relative energy (E_{rel}) is given for the lowest energy isomer. For each n, second line correspond to the case with two Y atoms. The energies are given in eV and the magnetic moment in μ_B

	Ground state					Lowest energy	
n	AE	ΔE	E_{xs}	E_{gap}	μ	μ	E_{rel}
1	1.370		0.903	0.365	1	3	1.024
	3.281		0.226	0.500	2	4	0.006
2	2.621	1.251	0.724	0.471	2	0	0.259
	4.743	1.462	0.035	0.476	1	3	0.078
3	4.007	1.385	0.786	0.699	3	1	0.115
	6.818	2.074	0.574	0.024	2	0	0.343
4	5.441	1.434	0.218	0.484	2	0	0.102
	8.401	1.584	0.435	0.397	1	3	0.385
5	6.961	1.520	0.073	0.615	1	3	0.204
	9.978	1.576	0.340	0.253	2	0	0.174
6	8.611	1.651	0.000	0.503	0	2	0.154
	11.396	1.418	0.460	0.280	3	1	0.011
7	9.931	1.319	0.495	0.403	1	3	0.307
	12.666	1.270	0.090	0.340	2	0	0.042
8	11.400	1.469	0.525	0.452	2	0	0.130
	14.099	1.433	0.041	0.408	1	3	0.130
9	12.825	1.425	0.171	0.318	1	3	0.292
	15.407	1.307	0.125	0.359	2	0	0.099
10	14.173	1.348	0.185	0.307	2	0	0.013
	16.899	1.492	0.190	0.359	3	1	0.019
11	15.664	1.491	0.052	0.397	1	3	0.041
	18.685	1.786	0.101	0.248	2	0	0.146
12	17.164	1.500	0.400	0.207	4	2	0.102
	20.381	1.697	0.043	0.340	1	3	0.406
13	18.695	1.530	0.199	0.386	3	1	0.047
14	20.297	1.602	0.000	0.125	0	2	0.199
15	22.114	1.817	0.095	0.272	1	3	0.681
16	23.849	1.735	0.000	0.865	0	2	0.700
17	24.786	0.937	0.190	0.190	1	3	1.002
18	26.006	1.219	0.000	0.509	0	4	0.385
19	27.015	1.009	0.324	0.324	1	3	0.404
20	28.117	1.102	0.000	0.313	0	2	0.061
21	29.522	1.405	0.043	0.237	1	3	0.072
22	30.528	1.006	0.326	0.326	2	4	0.043
23	32.159	1.631	0.242	0.242	1	3	0.214
24	33.561	1.402	0.000	0.345	0	2	0.185

Table S2 Ground state superorbital configurations for neutral YLi_n ($n = 1-24$) and Y_2Li_n ($n = 1-12$) clusters, and the charged YLi_n^+ ($n = 1-24$) and $Y_2Li_n^+$ ($n = 1-12$) clusters under study

n	YLi_n	YLi_n^+	Y_2Li_n	$Y_2Li_n^+$
1	$1S^2 1P_\alpha^1 1D_\alpha^1$	$1S^2 1P_\alpha^1$	$1S^2 1P_\alpha^3 1P_\beta^2$	$1S^2 1P_\alpha^3 1P_\beta^1$
2	$1S^2 1D_\alpha^1 1P_\alpha^1 1P_\beta^1$	$1S^2 1D_\alpha^1 1P_\alpha^1$	$1S^2 1P^6$	$1S^2 1P_\alpha^3 1P_\beta^2$
3	$1S^2 1P_\alpha^3 1P_\beta^1$	$1S^2 1P_\alpha^3$	$1S^2 1P^6 1D_\alpha^1$	$1S^2 1P_\alpha^3 1P_\beta^2 1D_\alpha^1$
4	$1S^2 1P_\alpha^3 1P_\beta^2$	$1S^2 1P_\alpha^3 1P_\beta^1$	$1S^2 1P^6 1D_\alpha^2$	$1S^2 1P^6 1D_\alpha^1$
5	$1S^2 1P^6$	$1S^2 1P_\alpha^3 1P_\beta^2$	$1S^2 1P^6 1D_\alpha^3$	$1S^2 1P^6 1D_\alpha^2$
6	$1S^2 1P^6 1D_\alpha^1$	$1S^2 1P^6$	$1S^2 1P^6 1D_\alpha^3 1D_\beta^1$	$1S^2 1P^6 1D_\alpha^3$
7	$1S^2 1P^6 1D_\alpha^2$	$1S^2 1P^6 1D_\alpha^1$	$1S^2 1P^6 1D_\alpha^3 1D_\beta^2$	$1S^2 1P^6 1D_\alpha^3 1D_\beta^1$
8	$1S^2 1P^6 1D_\alpha^2 1D_\beta^1$	$1S^2 1P^6 1D_\alpha^2$	$1S^2 1P^6 1D_\alpha^4 1D_\beta^2$	$1S^2 1P^6 1D_\alpha^3 1D_\beta^2$
9	$1S^2 1P^6 1D^4$	$1S^2 1P^6 1D_\alpha^2 1D_\beta^1$	$1S^2 1P^6 1D_\alpha^5 1D_\beta^2$	$1S^2 1P^6 1D_\alpha^4 1D_\beta^2$
10	$1S^2 1P^6 1D_\alpha^3 1D_\beta^2$	$1S^2 1P^6 1D_\alpha^3 1D_\beta^1$	$1S^2 1P^6 1D^8$	$1S^2 1P^6 1D_\alpha^5 1D_\beta^2$
11	$1S^2 1P^6 1D_\alpha^4 1D_\beta^2$	$1S^2 1P^6 1D_\alpha^3 1D_\beta^2$	$1S^2 1P^6 1D_\alpha^5 1D_\beta^4$	$1S^2 1P^6 1D_\alpha^5 1D_\beta^3$
12	$1S^2 1P^6 1D_\alpha^5 1D_\beta^2$	$1S^2 1P^6 1D_\alpha^5 1D_\beta^1$	$1S^2 1P^6 1D^{10}$	$1S^2 1P^6 1D_\alpha^5 1D_\beta^4$
13	$1S^2 1P^6 1D_\alpha^5 1D_\beta^3$	$1S^2 1P^6 1D_\alpha^5 1D_\beta^2$		
14	$1S^2 1P^6 1D_\alpha^5 1D_\beta^4$	$1S^2 1P^6 1D^8$		
15	$1S^2 1P^6 1D^{10}$	$1S^2 1P^6 1D_\alpha^5 1D_\beta^4$		
16	$1S^2 1P^6 1D^{10} 2S_\alpha^1$	$1S^2 1P^6 1D^{10}$		
17	$1S^2 1P^6 1D^{10} 2S^2$	$1S^2 1P^6 1D^{10} 2S_\alpha^1$		
18	$1S^2 1P^6 1D^{10} 1F_\alpha^1 1F_\beta^1 2S_\alpha^1$	$1S^2 1P^6 1D^{10} 1F^2$		
19	$1S^2 1P^6 1D^{10} 2S^2 1F^2$	$1S^2 1P^6 1D^{10} 2S^2 1F_\alpha^1$		
20	$1S^2 1P^6 1D^{10} 2S^2 1F_\alpha^2 1F_\beta^1$	$1S^2 1P^6 1D^{10} 2S^2 1F^2$		
21	$1S^2 1P^6 1D^{10} 1F_\alpha^3 1F_\beta^2 2S_\alpha^1$	$1S^2 1P^6 1D^{10} 1F_\alpha^3 1F_\beta^2$		
22	$1S^2 1P^6 1D^{10} 1F_\alpha^3 1F_\beta^3 2S_\alpha^1$	$1S^2 1P^6 1D^{10} 1F_\alpha^3 1F_\beta^2 2S_\alpha^1$		
23	$1S^2 1P^6 1D^8 1F^2 1D^2 1F^4 2S^2$	$1S^2 1P^6 1D_\alpha^4 1D_\beta^4 1F_\alpha^1 1F_\beta^1$		
		$1D_\alpha^1 1D_\beta^1 1F_\alpha^2 1F_\beta^2 2S_\alpha^1$		
24	$1S^2 1P^6 1D^{10} 2S^2 1F_\alpha^5 1F_\beta^2$	$1S^2 1P^6 1D^8 1F^2 1D^2 1F^4 2S^2$		

Table S3 Cartesian coordinates of the YLi cluster

Energy: -45.80041			
Multiplicity: 3			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.113904

Table S4 Cartesian coordinates of the YLi_2 cluster

Energy: -53.33777			
Multiplicity: 2			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.287104
Li	2.519105	0.000000	2.111643

Table S5 Cartesian coordinates of the YLi_3 cluster

Energy: -60.88328			
Multiplicity: 3			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.213408
Li	2.519891	0.000000	1.996074
Li	0.976556	-2.330523	1.987543

Table S6 Cartesian coordinates of the YLi_4 cluster

Energy: -68.42978			
Multiplicity: 2			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.184437
Li	2.604989	0.000000	1.939947
Li	0.861556	2.300006	2.033438
Li	-1.963004	1.712432	1.935585

Table S7 Cartesian coordinates of the YLi_5 cluster

Energy: -75.97492			
Multiplicity: 1			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.154598
Li	2.731973	0.000000	1.570342
Li	1.575470	2.231541	2.727397
Li	-0.912486	2.576616	1.571898
Li	1.817957	2.569250	-0.008223

Table S8 Cartesian coordinates of the YLi_6 cluster

Energy: -83.52426			
Multiplicity: 2			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.151338
Li	2.599418	0.000000	1.788474
Li	1.042560	2.417919	1.979114
Li	-1.796088	1.934152	1.803882
Li	2.506828	1.932136	-0.458730
Li	-0.253974	3.178579	-0.486793

Table S9 Cartesian coordinates of the YLi_7 cluster

Energy: -91.06322			
Multiplicity: 3			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.167008
Li	1.572784	0.000000	-2.838192
Li	1.048227	-2.431560	1.759649
Li	2.614010	-0.013057	1.907005
Li	2.731922	-1.500222	-0.603315
Li	1.076534	2.421002	1.765096
Li	2.753623	1.481419	-0.602456

Table S10 Cartesian coordinates of the YLi_8 cluster

Energy: -98.61077			
Multiplicity: 2			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.124059
Li	3.041028	0.000000	-0.714269
Li	2.214585	-1.452354	1.815449
Li	2.274973	1.455730	1.736436
Li	-0.288403	2.676895	1.698799
Li	1.582832	-2.676957	-0.670926
Li	1.660100	2.721083	-0.747988
Li	-0.339183	-2.722176	1.793383

Table S11 Cartesian coordinates of the YLi_9 cluster

Energy: -106.15818			
Multiplicity: 1			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.120862
Li	2.956442	0.000000	-0.999616
Li	2.421144	-1.123038	1.732116
Li	1.596656	-2.658563	-0.705804
Li	-0.146099	-2.664697	1.733376
Li	-1.388683	-2.609553	-0.999331
Li	2.204990	1.655614	1.580809
Li	-2.498147	-1.168643	1.582134
Li	0.690876	-1.165061	-2.880308

Table S12 Cartesian coordinates of the YLi_{10} cluster

Energy: -113.70363			
Multiplicity: 2			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.112168
Li	3.086608	0.000000	-0.793577
Li	2.294688	-1.439297	1.691240
Li	2.149717	1.533695	1.782896
Li	1.615961	2.580938	-0.950285
Li	1.521145	-2.491315	-1.075964
Li	1.047778	0.302901	-2.914435
Li	-0.474758	2.798194	1.270397
Li	-1.008239	2.451688	-1.834322
Li	-0.126251	-2.788702	1.610381

Table S13 Cartesian coordinates of the YLi_{11} cluster

Energy: -121.25287			
Multiplicity: 3			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.114050
Li	2.701044	0.000000	1.539260
Li	-2.021989	1.780927	1.559964
Li	2.337374	1.802149	-0.981485
Li	0.999317	-2.408667	1.706859
Li	0.320027	0.920205	-2.961997
Li	-0.582762	2.899951	-0.956390
Li	2.644741	-1.130404	-1.195158
Li	-2.338691	-1.156511	1.707653
Li	-2.748869	0.895708	-1.167511
Li	0.958964	2.536364	1.678684

Table S14 Cartesian coordinates of the YLi_{12} cluster

Energy: -128.80121			
Multiplicity: 4			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.040451
Li	0.000000	0.018252	-3.039814
Li	-0.636805	-2.627101	1.390257
Li	-2.693089	-0.228318	1.392095
Li	0.635690	2.634453	-1.382258
Li	2.695327	0.234746	-1.386172
Li	2.272601	-1.451072	1.464296
Li	-2.272867	1.461804	-1.457016
Li	-1.105564	2.467084	1.467076
Li	1.112187	-2.459846	-1.470929
Li	2.121790	1.831141	1.248436
Li	-2.127791	-1.826362	-1.242336

Table S15 Cartesian coordinates of the YLi_{13} cluster

Energy: -136.35398			
Multiplicity: 3			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	2.980566
Li	0.000000	0.268687	-3.039772
Li	-2.946678	-0.124096	1.115565
Li	2.945541	0.015224	1.123598
Li	-2.511099	1.185810	-1.472727
Li	2.457457	1.304644	-1.464915
Li	1.477681	2.519227	1.279887
Li	-1.599207	2.445324	1.276117
Li	-0.065521	2.841275	-1.362913
Li	-1.392569	-2.420843	1.579574
Li	1.502988	-2.355633	1.577502
Li	-2.167031	-1.769034	-1.414850
Li	2.254321	-1.661879	-1.410788

Table S16 Cartesian coordinates of the YLi_{14} cluster

Energy: -143.91667			
Multiplicity: 2			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	2.997817
Li	0.000000	-0.002353	-2.998133
Li	1.541397	-2.306817	-1.512549
Li	-0.125959	2.775236	1.506584
Li	-2.526500	1.192508	1.482949
Li	-1.326678	-2.477948	-1.460599
Li	2.832068	0.254714	-1.417663
Li	2.442578	1.504046	1.383784
Li	-2.385221	-1.669544	1.324447
Li	-2.937021	-0.103420	-1.280742
Li	1.285595	2.682998	-1.216169
Li	2.660269	-1.376362	1.176590
Li	0.198883	-3.007801	1.131937
Li	-1.655589	2.526330	-1.114546

Table S17 Cartesian coordinates of the YLi_{15} cluster

Energy: -151.47513			
Multiplicity: 1			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.075357
Li	2.662434	0.000000	-1.537289
Li	-2.662376	-0.002313	-1.536606
Li	-0.000663	1.377075	-2.911943
Li	0.000016	-1.378365	-2.911759
Li	-2.520955	1.376038	1.453573
Li	-2.519027	-1.378770	1.455703
Li	2.518732	1.379109	1.454418
Li	2.520655	-1.376165	1.454285
Li	-1.514580	2.749367	-0.875284
Li	0.001771	-2.753510	1.746710
Li	1.515157	-2.748340	-0.875122
Li	1.511713	2.750304	-0.874895
Li	-0.001765	2.753573	1.747829
Li	-1.513266	-2.749733	-0.874789

Table S18 Cartesian coordinates of the YLi_{16} cluster

Energy: -159.01918			
Multiplicity: 2			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.128304
Li	2.952390	0.000000	-1.036688
Li	-1.471732	2.554501	-1.044847
Li	-1.471830	-2.552823	-1.046551
Li	-0.022755	2.819481	1.740693
Li	-2.434878	1.431840	1.731418
Li	1.630574	2.822739	-0.595062
Li	0.835980	1.431060	-2.871910
Li	-1.646647	0.007573	-2.875071
Li	-3.253208	-0.005477	-0.603530
Li	-2.434802	-1.428952	1.740372
Li	-0.025061	-2.826571	1.730397
Li	2.450089	-1.391555	1.740053
Li	2.457613	1.391433	1.738044
Li	1.633964	-2.819929	-0.601009
Li	0.827816	-1.428708	-2.873133

Table S19 Cartesian coordinates of the YLi_{17} cluster

Energy: -166.55270			
Multiplicity: 1			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.175112
Li	2.785055	0.000000	1.524552
Li	-0.987954	-2.608950	1.519831
Li	1.803028	-2.609170	-0.127487
Li	-0.388965	3.161334	-0.669233
Li	-1.654746	-0.213663	-2.798557
Li	-2.827916	1.478999	-0.667597
Li	0.781066	1.472564	-2.803666
Li	1.613421	-2.343041	2.730459
Li	-1.619473	2.335176	1.857944
Li	-2.690923	-0.252824	1.987945
Li	1.181379	2.430617	1.986509
Li	2.411281	2.339328	-0.534601
Li	3.038130	-0.254994	-1.402283
Li	-3.041729	-1.433673	-0.534086
Li	-0.833907	-2.933020	-1.404537
Li	0.995142	-1.439076	-2.921034

Table S20 Cartesian coordinates of the YLi_{18} cluster

Energy: -174.08305			
Multiplicity: 2			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.131870
Li	1.807404	0.000000	-2.560616
Li	0.538880	-2.643306	1.596766
Li	1.257663	2.683678	-1.011907
Li	-3.000720	-0.062733	-0.955761
Li	3.027099	-1.182448	0.228901
Li	3.843326	1.241998	-0.798885
Li	2.535956	1.239169	1.621626
Li	2.753284	-1.162478	2.981996
Li	1.195165	-2.720666	-1.372663
Li	0.083396	2.739197	1.791572
Li	-0.769349	1.479215	-2.841255
Li	-1.743147	2.764471	-0.501996
Li	-0.905497	-1.354285	-2.880927
Li	-1.617745	-2.843600	-0.555672
Li	-2.235430	-1.550006	1.880533
Li	-2.455573	1.270623	1.826687
Li	5.390060	0.100466	1.750251

Table S21 Cartesian coordinates of the YLi_{19} cluster

Energy: -181.61820			
Multiplicity: 1			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.092261
Li	2.680434	0.000000	1.543685
Li	-2.271839	1.953528	-0.939055
Li	0.314998	1.961354	-2.435824
Li	-0.619728	-2.915021	-1.083106
Li	1.002927	-2.534212	1.724485
Li	-1.810364	-2.146353	1.760688
Li	2.438640	-2.136608	-0.694244
Li	-1.677342	-0.018722	-2.905521
Li	1.021390	-1.008614	-2.913430
Li	-3.029869	-1.018384	-0.574250
Li	1.736958	2.780534	0.297109
Li	-0.623782	2.778230	1.658263
Li	1.747596	2.521264	3.031749
Li	-2.646611	0.678394	1.812496
Li	2.890555	0.691320	-1.384459
Li	-0.501938	4.228178	-0.851685
Li	-2.043568	3.334935	-3.517100
Li	1.022661	5.328966	1.794022

Table S22 Cartesian coordinates of the YLi_{20} cluster

Energy: -189.15416			
Multiplicity: 2			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.281257
Li	3.055756	0.000000	-0.712563
Li	-0.768844	-2.554956	1.659098
Li	-3.209725	0.302364	-0.717670
Li	-2.598865	-0.091514	1.972309
Li	-3.704343	-2.118200	0.527281
Li	-1.408840	0.139680	-2.948367
Li	-3.301333	2.469314	1.072185
Li	-4.500703	3.143834	-1.195505
Li	-1.401190	2.622056	-1.130710
Li	-0.551501	2.602358	1.743040
Li	1.390406	3.013892	-0.296048
Li	1.142597	1.516419	-2.656588
Li	1.135704	-1.364135	-2.793142
Li	-1.386498	-2.431475	-1.356431
Li	2.277233	1.392041	1.909248
Li	2.147229	-1.491785	1.926619
Li	1.436026	-2.895045	-0.402321
Li	-5.602769	0.608750	0.772171
Li	-2.193763	4.998928	0.144516

Table S23 Cartesian coordinates of the YLi_{21} cluster

Energy: -196.70029			
Multiplicity: 3			
Atom	x	y	z
Li	0.000000	0.000000	0.000000
Li	0.000000	0.000000	2.686523
Li	2.571513	0.000000	0.851906
Li	-1.466455	1.511358	-1.671485
Li	-1.378467	-1.906598	-1.404415
Li	-2.552239	0.111753	0.972742
Li	1.492752	2.062270	-1.108649
Li	-0.672562	2.478574	0.975566
Li	-0.603693	-2.517756	1.251330
Y	1.935540	-2.802390	-0.751596
Li	4.692460	-3.919344	-1.700251
Li	-0.373717	-4.881151	-1.225262
Li	2.167432	-2.399978	2.410237
Li	3.912023	-0.416935	-1.728870
Li	3.084148	-2.238929	-3.761124
Li	4.796324	-1.895889	0.625040
Li	1.026220	-0.331768	-2.641370
Li	3.885846	-4.566503	1.260791
Li	2.547757	-6.087492	-0.691529
Li	2.202195	-4.948691	-3.195004
Li	0.188008	-2.972197	-3.602587
Li	0.932384	-4.967456	1.484371

Table S24 Cartesian coordinates of the YLi_{22} cluster

Energy: -204.24567			
Multiplicity: 2			
Atom	x	y	z
Li	0.000000	0.000000	0.000000
Li	0.000000	0.000000	4.610408
Y	2.358346	0.000000	2.302700
Li	-0.738033	-1.351851	2.300054
Li	1.408685	-2.685717	3.806914
Li	1.969711	2.160864	4.722094
Li	1.452353	-2.715558	0.857907
Li	5.314237	2.678022	2.290734
Li	4.789067	4.049561	4.569916
Li	4.789099	4.078841	0.025671
Li	4.659682	1.028137	0.167144
Li	4.668651	1.015683	4.412616
Li	2.616491	-0.650040	-0.972354
Li	-0.091844	1.957822	2.305320
Li	6.217849	-0.020081	2.295468
Li	7.480066	2.647130	0.763440
Li	2.635081	-0.633915	5.577487
Li	4.366756	-2.065804	3.705931
Li	2.725151	3.339387	2.298890
Li	6.445778	5.105955	2.305186
Li	4.398766	-2.036104	0.866729
Li	7.485030	2.637884	3.815534
Li	1.964282	2.166210	-0.123899

Table S25 Cartesian coordinates of the YLi_{23} cluster

Energy: -211.78860			
Multiplicity: 1			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.129251
Li	2.814306	0.000000	1.374235
Li	0.338088	-1.231952	-2.883457
Li	-2.741064	-1.223906	-0.939944
Li	1.755076	2.628931	-0.152216
Li	-0.916691	2.651833	1.506424
Li	1.624327	2.472077	2.594864
Li	-0.413371	-3.186252	-0.659547
Li	-1.662067	-2.282047	1.784762
Li	-2.719171	0.334499	1.918261
Li	-2.819945	1.753441	-0.480527
Li	-1.800118	0.916042	-2.891129
Li	0.817328	1.726764	-2.766814
Li	2.927593	0.353761	-1.604011
Li	-0.813852	3.546590	-1.373117
Li	-1.174066	6.181452	-2.039818
Li	2.337306	-2.272197	-0.736928
Li	1.192584	-2.440025	1.884533
Li	-2.642895	4.906523	0.231065
Li	1.477597	4.832797	-2.314789
Li	-3.283581	3.977497	-2.582659
Li	-0.789918	3.970695	-4.140804
Li	0.403774	5.252623	0.566413

Table S26 Cartesian coordinates of the YLi_{24} cluster

Energy: -219.33082			
Multiplicity: 4			
Atom	x	y	z
Li	2.793740	3.803472	0.391262
Li	2.963148	-2.325233	2.696200
Li	-2.973626	2.371030	0.108376
Li	-2.576310	-2.777307	-0.459632
Li	1.976494	1.362221	-0.368911
Li	3.288852	-3.445854	-0.199040
Li	-0.105609	3.041259	-1.086726
Li	-2.023188	-1.931043	2.407579
Li	3.167292	1.018168	2.123147
Li	0.229151	-3.050229	1.026284
Li	0.214212	2.361321	1.687685
Li	0.512896	-0.400037	2.710280
Li	-2.044423	1.650647	-2.685720
Li	2.117506	-1.129341	0.473514
Li	0.684973	0.462799	-2.759378
Li	-3.983427	-0.121539	-1.597895
Li	2.831889	2.686432	-2.519188
Li	0.668609	-2.329705	-1.722113
Li	-4.085393	-0.454875	1.139039
Li	4.911852	-1.101457	0.756536
Li	4.768619	1.700270	-0.439449
Li	-2.185644	1.067465	2.774476
Y	-1.063381	-0.079362	-0.096064
Li	3.417627	-0.616856	-1.927605
Li	-1.761840	-1.337532	-3.056324

Table S27 Cartesian coordinates of the Y_2Li cluster

Energy: -84.15872			
Multiplicity: 2			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Y	0.000000	0.000000	3.201230
Li	2.729101	0.000000	1.593055

Table S28 Cartesian coordinates of the Y_2Li_2 cluster

Energy: -91.71077			
Multiplicity: 1			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Y	0.000000	0.000000	3.194763
Li	2.697361	0.000000	1.594187
Li	1.068785	2.480639	1.598267

Table S29 Cartesian coordinates of the Y_2Li_3 cluster

Energy: -99.26120			
Multiplicity: 2			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Y	0.000000	0.000000	3.219030
Li	2.704859	0.000000	1.612884
Li	1.156340	-2.496877	1.610637
Li	1.157606	2.496870	1.610879

Table S30 Cartesian coordinates of the Y_2Li_4 cluster

Energy: -106.80760			
Multiplicity: 3			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Y	0.000000	0.000000	3.226185
Li	2.763157	0.000000	1.614236
Li	1.175096	2.500642	1.615083
Li	-1.745056	2.108929	1.611865
Li	1.165865	-2.476486	1.612197

Table S31 Cartesian coordinates of the Y_2Li_5 cluster

Energy: -114.36121			
Multiplicity: 4			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Y	0.000000	0.000000	3.282194
Li	2.680729	0.000000	1.640162
Li	-2.159197	-1.596912	1.643779
Li	0.807642	2.560795	1.642684
Li	0.842097	-2.547976	1.641024
Li	-2.189733	1.553843	1.641305

Table S32 Cartesian coordinates of the Y_2Li_6 cluster

Energy: -121.90711			
Multiplicity: 3			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Y	0.000000	0.000000	3.189013
Li	2.785948	0.000000	1.594065
Li	-2.786286	0.001664	1.594846
Li	1.455474	-2.494431	1.598588
Li	-1.446426	-2.473644	1.594785
Li	-1.455087	2.497289	1.597700
Li	1.445214	2.478743	1.594781

Table S33 Cartesian coordinates of the Y_2Li_7 cluster

Energy: -129.44566			
Multiplicity: 2			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Li	0.000000	0.000000	4.211889
Y	2.355987	0.000000	2.097952
Li	-0.009514	-2.289944	2.302957
Li	-0.011504	2.287445	2.304098
Li	3.054463	0.001195	-1.023000
Li	1.996371	2.508101	0.118689
Li	2.003791	-2.507663	0.122039
Li	-2.056446	-0.004200	2.434576

Table S34 Cartesian coordinates of the Y_2Li_8 cluster

Energy: -136.99085			
Multiplicity: 3			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Y	0.000000	0.000000	3.171342
Li	2.882933	0.000000	1.394191
Li	-2.868880	0.003322	1.638231
Li	2.736378	1.472118	-1.067071
Li	2.733004	-1.479397	-1.062921
Li	1.445982	2.481636	1.454133
Li	-1.426114	2.463541	1.532413
Li	1.437908	-2.485736	1.455577
Li	-1.432811	-2.460378	1.532509

Table S35 Cartesian coordinates of the Y_2Li_9 cluster

Energy: -144.53177			
Multiplicity: 4			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Y	0.000000	0.000000	3.237304
Li	2.728909	0.000000	1.527685
Li	0.632356	2.654222	1.528089
Li	1.065788	-2.524332	1.421658
Li	-2.207882	1.621802	1.420604
Li	2.431362	1.919174	-0.758938
Li	-2.118743	-1.664549	1.644980
Li	-0.483084	2.888677	-1.171979
Li	2.697083	-1.141973	-1.170463
Li	1.079182	0.849443	-2.923501

Table S36 Cartesian coordinates of the Y_2Li_{10} cluster

Energy: -152.08424			
Multiplicity: 1			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Y	0.000000	0.000000	3.071102
Li	2.738900	0.000000	1.205788
Li	-2.217029	-1.606099	1.204216
Li	0.846325	2.603830	1.206421
Li	-2.214784	1.609191	1.204534
Li	0.844568	-2.602875	1.204064
Li	-2.917162	0.002079	-1.213219
Li	-0.902531	-2.774943	-1.211417
Li	2.360308	-1.715074	-1.210857
Li	2.361352	1.713827	-1.209595
Li	-0.900834	2.773464	-1.211874

Table S37 Cartesian coordinates of the Y_2Li_{11} cluster

Energy: -159.64730			
Multiplicity: 2			
Atom	x	y	z
Li	0.000000	0.000000	0.000000
Li	0.000000	0.000000	3.235070
Y	2.539055	0.000000	1.582651
Li	5.194896	-0.415642	3.060260
Li	5.132514	-0.425737	-0.065690
Y	1.189540	2.741356	1.551612
Li	0.858920	-2.563598	1.656079
Li	2.722805	1.368271	-1.050353
Li	2.585233	-1.750938	4.084068
Li	4.516275	2.236597	1.451154
Li	3.926428	-2.766727	1.532533
Li	2.385830	-1.784864	-0.948989
Li	2.963885	1.467286	4.194771

Table S38 Cartesian coordinates of the Y_2Li_{12} cluster

Energy: -167.20644			
Multiplicity: 1			
Atom	x	y	z
Y	0.000000	0.000000	0.000000
Y	0.000000	0.000000	3.018251
Li	2.524083	0.000000	-1.685453
Li	-0.183110	0.042392	-3.116476
Li	0.540222	-2.527129	-1.679627
Li	-1.378982	-2.526750	1.091922
Li	-2.854259	0.073304	1.132134
Li	-2.334976	-1.448601	-1.524124
Li	-1.222300	2.595184	1.106129
Li	-2.278941	1.574825	-1.498332
Li	1.680731	2.382963	1.107827
Li	0.621763	2.553741	-1.633254
Li	2.936600	-0.116255	1.237368
Li	1.503170	-2.509382	1.112045