Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplemental material (cartesian coordinates of all studied clusters in Angstrom) for: Quantum Monte Carlo study on electron correlation effects in small aluminum hydride clusters

J. Higino Damasceno Jr., J.N. Teixeira Rabelo and Ladir Cândido

Aluminum clusters

Al_2 (Singlet)

Al	-0.008315	-0.765020	-0.533412
Al	0.015697	1.855467	-0.351997

Al_4 (Singlet)

Al	-4.468992	-1.398344	-0.598850
Al	-4.175428	1.291267	0.620891
Al	-6.779719	0.883245	1.144442
Al	-5.676123	1.257385	-1.273258

Al_6 (Singlet)

Al	1.898485	0.004080	0.540821
Al	-0.600613	-1.494170	1.147565
Al	-1.898018	-0.003856	-0.540984
Al	0.600171	1.494492	-1.147985
Al	0.607918	-1.488135	-1.152211
Al	-0.607840	1.487625	1.152025

Al_7 (Dublet)

Al	0.526165	0.000741	1.699623
Al	-1.504965	1.372396	0.792266
Al	-1.505760	0.000336	-1.585204
Al	0.526263	-1.469550	-0.849516
Al	-1.503847	-1.372936	0.792575
Al	0.526929	1.469433	-0.848404
Al	2.598647	-0.000349	0.000936

Al_8 (Singlet)

Al	0.880642	1.009027	-1.275474
Al	-1.238009	2.034584	-1.238589
Al	1.267816	-2.023831	1.258288
Al	1.779382	-1.573257	-1.247251
Al	1.159157	0.715827	1.251149
Al	-0.905637	-1.021053	-1.249444
Al	-1.135640	-0.707493	1.277807
Al	-1.807622	1.566125	-1.251363

Al_{13} (Dublet)

Al	-0.007693	-0.000344	-0.031465
Al	-0.077392	1.481924	2.184500
Al	-0.071856	-1.479483	2.186722
Al	0.058527	1.477881	-2.250195
Al	0.063992	-1.481377	-2.248140
Al	1.428458	2.306608	0.010682
Al	1.437007	-2.301757	0.014157
Al	-1.451018	2.300297	-0.079061
Al	-1.442722	-2.306119	-0.075778
Al	2.321324	0.005081	1.269943
Al	2.279493	0.002850	-1.499874
Al	-2.292244	-0.003519	1.435114
Al	-2.334914	-0.005403	-1.334290

Al_{14} (Singlet)

Al	-0.001849	2.252713	-1.473218
Al	-2.358920	0.716329	-1.378189
Al	-1.543892	-1.922939	-1.218862
Al	1.262677	-2.011058	-1.229901
Al	2.247927	0.568135	-1.383953
Al	-1.435526	1.957165	0.973324
Al	-2.387405	-0.627578	1.112364
Al	-0.153184	-2.303562	1.192035
Al	2.192568	-0.793608	1.103596
Al	1.427388	1.849219	0.976001
Al	-0.074539	-0.020261	-0.129740
Al	-0.085233	-0.152158	-2.819609
Al	-0.068335	0.090353	2.573592
Al	0.093917	4.384873	0.504124

Aluminum hydride clusters

AlH^+ (Dublet)

Al	0.026699	0.000000	0.000000
H	1.653301	0.000000	0.000000

AlH (Singlet)

Al	0.001082	0.000000	0.000000
H	1.678918	0.000000	0.000000

AlH^- (Dublet)

Al	-0.017397	0.000000	0.000000
H	1.697397	0.000000	0.000000

AlH_2^+ (Singlet)

Al	0.000000	0.000000	0.000000
H	1.561000	0.000000	0.000000
H	-1.561000	0.000000	0.000000

AlH_2 (Dublet)

Al	0.000000	-0.194964	0.000000
H	1.383604	0.630988	0.000000
H	-1.383604	0.630988	0.000000

AlH_2^- (Singlet)

Al	0.000000	-0.422300	0.000000
H	1.250572	0.744656	0.000000
H	-1.250572	0.744656	0.000000

AlH_3^+ (Dublet)

Al	0.000181	-0.571063	0.000000
H	0.902324	0.848584	0.000000
H	-0.000016	-2.125989	0.000000
H	-0.902490	0.848468	0.000000

AlH_3 (Singlet)

Al	0.000000	-0.250025	0.000000
H	1.379402	0.546453	0.000000
H	0.000000	-1.842882	0.000000
H	-1.379402	0.546453	0.000000

AlH_3^- (Dublet)

Al	-0.007485	-0.258617	0.540406
H	1.360173	0.531337	0.092647
H	-0.005088	-1.833279	0.076484
H	-1.370825	0.531753	0.080516

$Al_2H_6^+$ (Dublet)

Al	-0.007389	-0.747322	-0.532267
Al	0.015916	1.840097	-0.353008
H	0.017210	0.465701	0.712390
H	-0.003385	0.625654	-1.597811
H	1.419212	2.651021	-0.309692
H	-1.377748	2.665776	-0.283868
H	-1.414328	-1.552673	-0.575228
H	1.377980	-1.586576	-0.602214

Al_2H_6 (Singlet)

Al	-0.008612	-0.764507	-0.533357
Al	0.015523	1.854926	-0.352069
H	0.013860	0.465445	0.710738
H	-0.006669	0.624971	-1.596166
H	1.444743	2.537046	-0.317718
H	-1.401103	2.561026	-0.290870
H	-1.438055	-1.446164	-0.567672
H	1.407782	-1.471067	-0.594585

$Al_2H_6^-$ (Dublet)

Al	-0.004280	-0.783687	-0.242283
Al	0.012769	2.352538	-1.131828
H	-0.002830	-0.332281	1.312469
H	-0.004273	0.640744	-1.248383
H	1.398523	2.750117	-0.385665
H	-1.360939	2.776256	-0.377740
H	-1.367198	-1.518963	-0.733252
H	1.355697	-1.523043	-0.735017

$Al_4H_6^+$ (Dublet)

Al	-4.692365	-1.006836	-0.479769
Al	-4.012043	1.229307	0.822980
Al	-6.579291	0.645991	1.028610
Al	-5.816440	1.162100	-1.483494
H	-7.182830	1.330085	-0.439070
H	-7.791773	0.322625	1.982115
H	-4.468520	-2.563223	-0.598718
H	-6.010155	2.095932	-2.739188
H	-3.366850	-0.312874	0.385529
H	-2.830855	2.179601	1.253804

Al_4H_6 (Singlet)

Al	-4.801576	-1.004506	-0.348576
Al	-4.035227	1.283491	0.666217
Al	-6.551870	0.495072	0.966316
Al	-5.711591	1.259496	-1.390734
H	-7.155776	1.317536	-0.433838
H	-7.797478	0.469120	1.961057
H	-4.353261	-2.499007	-0.674675
H	-6.123468	1.995928	-2.743336
H	-3.394705	-0.301337	0.380661
H	-2.826172	2.066914	1.349706

$Al_4H_6^-$ (Dublet)

Al	-4.871796	-1.020800	-0.378225
Al	-4.079226	1.348867	0.671221
Al	-6.509274	0.456397	1.021079
Al	-5.640295	1.248582	-1.421290
H	-7.114791	1.298472	-0.425015
H	-7.801211	0.457705	1.993313
H	-4.369214	-2.525923	-0.688913
H	-6.105656	2.004634	-2.772715
H	-3.436040	-0.283255	0.371645
H	-2.823620	2.098025	1.361698

$Al_6H_2^+$ (Dublet)

Al	0.099788	1.963888	0.046551
Al	1.393639	0.017144	1.384797
Al	-0.098886	-1.965332	0.060565
Al	-1.461079	-0.082382	-1.287844
Al	1.424277	0.075440	-1.330447
Al	-1.350827	-0.008235	1.426205
H	-0.123463	1.135719	-1.763297
H	0.073758	-1.145764	-1.760059

Al_6H_2 (Singlet)

Al	0.018885	1.922595	0.014981
Al	1.390921	0.009543	1.355050
Al	0.033519	-1.921118	0.026555
Al	1.489703	0.002413	-1.243601
Al	-1.424611	-0.008685	-1.264396
Al	-1.367611	-0.000308	1.331232
H	0.032023	1.121797	-1.760071
H	0.038928	-1.130287	-1.754428

$Al_6H_2^-$ (Dublet)

Al	-1.481928	-0.040218	1.349283
Al	-1.483648	-0.015532	-1.349929
Al	1.483648	-0.015532	-1.349929
Al	1.481928	-0.040218	1.349283
Al	0.000000	-1.829348	-0.016879
Al	0.000000	1.877161	0.015287
H	0.000000	0.997888	1.814395
H	0.000000	1.026622	-1.799448

Al_7H^+ (Dublet)

Al	0.545485	-0.162194	1.750468
Al	-1.465494	1.348075	0.778748
Al	-1.598245	0.050942	-1.585558
Al	0.566517	-1.392972	-0.805289
Al	-1.597437	-1.349097	0.838220
Al	0.543727	1.433805	-1.013348
Al	2.612008	-0.001021	-0.001987
H	4.193223	0.072463	0.040979

Al_7H (Singlet)

Al	0.534501	0.000078	1.719437
Al	-1.493218	1.359591	0.784906
Al	-1.493235	0.000122	-1.569652
Al	0.534779	-1.487202	-0.858871
Al	-1.492993	-1.359757	0.784724
Al	0.534746	1.487338	-0.858701
Al	2.537578	-0.000099	0.000395
H	4.137624	-0.000070	-0.000004

Al_7H^- (Dublet)

Al	0.616465	-0.028670	1.822027
Al	-1.420419	1.334334	0.793622
Al	-1.659268	-0.002461	-1.709872
Al	0.509444	-1.381817	-0.892574
Al	-1.453654	-1.322076	0.773379
Al	0.509889	1.380390	-0.909819
Al	2.541173	0.003666	0.129571
H	4.156153	0.016631	-0.004102

$Al_7H_3^+$ (Dublet)

Al	-0.695014	1.549518	0.005899
Al	1.443612	0.957036	1.455652
Al	1.704471	-1.354582	-0.004148
Al	-0.436041	-0.806122	-1.543499
Al	1.450944	0.974597	-1.437550
Al	-0.440475	-0.827709	1.532478
Al	-2.624430	-0.245188	-0.003579
H	-4.186185	-0.488553	-0.005557
H	2.898891	-2.388751	-0.016804
H	-2.378973	1.582971	0.012658

Al_7H_3 (Singlet)

Al	-0.685305	1.631517	0.007210
Al	1.385548	0.964293	1.383029
Al	1.615984	-1.466047	-0.007431
Al	-0.438813	-0.878188	-1.453884
Al	1.386969	0.976954	-1.371681
Al	-0.438940	-0.893878	1.446926
Al	-2.552229	-0.246943	-0.001131
H	-4.134300	-0.442570	-0.002547
H	2.966923	-2.303761	-0.012060
H	-2.369038	1.611841	0.007122

$Al_7H_3^-$ (Dublet)

Al	-0.488885	-0.615327	-1.519286
Al	1.632638	0.942295	-1.442208
Al	1.482384	0.830170	1.279902
Al	-0.568639	-0.738961	1.649686
Al	1.463298	-1.469374	0.001404
Al	-0.655925	1.621976	-0.011223
Al	-2.538446	-0.428229	0.099968
H	-4.143626	-0.553580	-0.046104
H	-1.321813	3.086393	-0.021015
H	2.164196	-2.916790	0.008280

$Al_8H_4^+$ (Dublet)

Al	0.555344	1.259245	-1.239140
Al	-0.532069	2.203509	1.017446
Al	0.532116	-2.204308	1.018011
Al	2.085705	-0.889558	-1.016960
Al	1.335903	0.341505	1.239276
Al	-0.555857	-1.260488	-1.240529
Al	-1.337068	-0.341737	1.240431
Al	-2.086142	0.890086	-1.017067
H	-3.413283	1.468056	-1.658459
H	3.413439	-1.465733	-1.657874
H	-0.880575	3.608813	1.657374
H	0.882483	-3.609389	1.658582

Al_8H_4 (Singlet)

Al	0.535374	1.234390	-1.208024
Al	-0.541877	2.189181	1.000187
Al	0.541360	-2.188174	0.999598
Al	2.070298	-0.897473	-0.999697
Al	1.307451	0.325663	1.207523
Al	-0.534688	-1.233122	-1.207136
Al	-1.306071	-0.325513	1.206822
Al	-2.069625	0.896593	-0.999443
H	-3.412027	1.416309	-1.687215
H	3.412077	-1.419161	-1.687946
H	-0.834039	3.598733	1.689023
H	0.831768	-3.597425	1.687398

$Al_8H_4^-$ (Dublet)

Al	0.581641	1.211333	-1.228018
Al	-0.656812	2.213558	0.925413
Al	0.656606	-2.213846	0.925746
Al	2.074873	-1.014686	-0.925651
Al	1.292605	0.374888	1.229303
Al	-0.581931	-1.211307	-1.228235
Al	-1.292570	-0.374583	1.229104
Al	-2.074588	1.014851	-0.925321
H	-3.424344	1.336513	-1.747086
H	3.424827	-1.336229	-1.747619
H	-0.751599	3.598172	1.746446
H	0.751290	-3.598661	1.747009

$Al_{13}H^+$ (Dublet)

Al	0.052675	-0.000465	-0.021373
Al	-0.113992	1.403957	2.213264
Al	-0.098325	-1.407101	2.212047
Al	0.068175	1.719506	-2.113028
Al	0.054532	-1.721608	-2.112939
Al	1.414074	2.365478	0.162199
Al	1.420844	-2.360449	0.150202
Al	-1.506304	2.308980	0.049253
Al	-1.507364	-2.307568	0.059951
Al	2.503021	0.004448	0.982759
Al	2.205932	-0.005943	-1.721425
Al	-2.442240	0.000162	1.210725
Al	-2.081871	0.002684	-1.503425
H	0.030848	-0.002081	3.318391

$Al_{13}H$ (Singlet)

Al	0.000705	0.000569	-0.021098
Al	-0.000487	1.414313	2.197374
Al	-0.000489	-1.414172	2.196720
Al	-0.000055	1.548479	-2.181749
Al	-0.000053	-1.548237	-2.181263
Al	1.460469	2.289780	0.038385
Al	1.459614	-2.289466	0.038211
Al	-1.460835	2.289347	0.038031
Al	-1.459987	-2.289037	0.037855
Al	2.386783	-0.000350	1.242829
Al	2.221499	-0.000299	-1.533801
Al	-2.386474	-0.000353	1.242539
Al	-2.221056	-0.000297	-1.533580
H	0.000369	-0.000278	3.306146

$Al_{13}H^-$ (Dublet)

Al	-0.000421	-0.001153	-0.020938
Al	0.123648	1.413628	2.187319
Al	-0.130478	-1.414448	2.188358
Al	-0.054091	1.564581	-2.145333
Al	0.058128	-1.566512	-2.145029
Al	1.559339	2.455636	-0.019214
Al	1.437045	-2.279105	0.118162
Al	-1.438153	2.279622	0.113060
Al	-1.561824	-2.454088	-0.023239
Al	2.384453	0.022435	1.210033
Al	2.205165	0.033099	-1.540295
Al	-2.385244	-0.020220	1.209402
Al	-2.204012	-0.032925	-1.541690
H	0.006447	-0.000552	3.296003

$Al_{14}H_2^+$ (Dublet)

Al	-0.039467	2.251096	-1.679288
Al	-2.366556	0.749867	-1.378000
Al	-1.551588	-1.896108	-1.222154
Al	1.321786	-1.909445	-1.193815
Al	2.264312	0.641435	-1.391375
Al	-1.632295	1.921185	1.039756
Al	-2.397980	-0.646749	1.150135
Al	-0.107322	-2.201629	1.245314
Al	2.217571	-0.772760	1.123123
Al	1.563921	1.826458	1.047219
Al	-0.090814	0.070291	-0.128345
Al	-0.053868	-0.162252	-2.851488
Al	-0.072144	0.163439	2.602400
Al	0.034896	3.900556	0.410803
H	0.137599	5.462053	0.662694
H	-2.340391	-3.133123	-1.835336

$Al_{14}H_2$ (Singlet)

Al	-0.084876	2.258811	-1.592205
Al	-2.363997	0.690765	-1.381254
Al	-1.596939	-1.921017	-1.252074
Al	1.290948	-1.923118	-1.193073
Al	2.206218	0.653296	-1.403267
Al	-1.576371	1.949463	0.963754
Al	-2.393055	-0.642979	1.091482
Al	-0.121005	-2.213711	1.212318
Al	2.197670	-0.754852	1.114875
Al	1.592738	1.873569	1.074108
Al	-0.055025	0.083677	-0.106270
Al	-0.103711	-0.170088	-2.818180
Al	-0.114389	0.173682	2.560747
Al	0.237387	3.930126	0.530606
H	0.070172	5.514071	0.624300
H	-2.298107	-3.237379	-1.824222

$Al_{14}H_2^-$ (Dublet)

Al	0.017241	2.287053	-1.570740
Al	-2.320078	0.732883	-1.352786
Al	-1.592920	-1.918610	-1.248272
Al	1.318143	-1.997461	-1.262546
Al	2.208986	0.610706	-1.361985
Al	-1.512696	1.970477	1.042804
Al	-2.367312	-0.618120	1.105567
Al	-0.156804	-2.303433	1.256160
Al	2.174086	-0.791739	1.094332
Al	1.558163	1.917208	1.061643
Al	-0.043147	0.048168	-0.103395
Al	-0.081337	-0.145868	-2.798521
Al	-0.073926	0.138761	2.535741
Al	0.119652	3.974487	0.466536
H	-0.016781	5.569159	0.581631
H	-2.343608	-3.209357	-1.844527