Supporting Information

for

Excess Electron in $LiAlH_4$ Clusters: Implication for Hydrogen Storage

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Table S1. The Coordinates and the NBO charge populations.

Complexes	Atom	Coordinates (Angstroms)			NBO Charges	Complexes	Atom	Coordinates (Angstroms)			NBO Charges
		X	Y	Z				X	Y	Z	
M_1	Al	0.000000	0.000000	0.391457	0.648	M_1^-	Al	0.000000	0.000000	0.399524	0.514
	H	0.000000	0.000000	1.967150	-0.303		H	0.000000	0.000000	2.000669	-0.335
	H	0.000000	1.392449	-0.514595	-0.423		H	0.000000	1.437440	-0.403115	-0.399
	H	-1.205896	-0.696225	-0.514595	-0.423		H	-1.244859	-0.718720	-0.403115	-0.399
	H	1.205896	-0.696225	-0.514595	-0.423		H	1.244859	-0.718720	-0.403115	-0.399
	Li	0.000000	0.000000	-1.837437	0.925		Li	0.000000	0.000000	-1.995046	0.018
M_2	H	0.791959	0.000000	1.202882	-0.489	M_2^-	H	1.217057	-0.720947	0.000000	-0.454
	H	0.791989	0.000000	-1.202867	-0.489		H	-1.217057	-0.720947	0.000000	-0.454
	H	-1.192442	-1.387780	-0.000016	-0.331		H	0.000000	1.279688	1.361591	-0.359
	H	-1.192442	1.387780	-0.000016	-0.331		H	0.000000	1.279688	-1.361591	-0.359
	Al	-0.411819	0.000000	0.000002	0.720		Al	0.000000	0.416546	0.000000	0.629
	Li	2.051527	0.000000	-0.000001	0.920		Li	0.000000	-2.177527	0.000000	-0.002
D_1	Al	-0.284811	0.675972	1.989618	0.632	D_2	Li	-1.594097	0.000000	0.000000	0.458
	H	-0.542598	1.277151	3.444156	-0.340		Li	1.594097	0.000000	0.000000	0.458
	H	1.266556	0.216099	1.664025	-0.417		Al	-4.171182	0.000000	0.000000	0.651
	H	-0.970272	-0.794017	1.684176	-0.417		Al	4.171182	0.000000	0.000000	0.651
	H	-0.770184	1.730592	0.815540	-0.452		H	-3.032463	0.000000	1.217788	-0.447
	Li	-0.661121	1.438567	-0.926429	0.495		H	3.032463	0.000000	1.217788	-0.447
	H	0.770184	-1.730592	-0.815540	-0.452		H	-3.032463	0.000000	-1.217788	-0.447
	Al	0.284811	-0.675972	-1.989618	0.632		H	3.032463	0.000000	-1.217788	-0.447
	H	0.542598	-1.277151	-3.444156	-0.340		H	-5.025262	1.364647	0.000000	-0.357
	Li	0.661121	-1.438567	0.926429	0.495		H	5.025262	-1.364647	0.000000	-0.357
	H	-1.266556	-0.216099	-1.664025	-0.417		H	-5.025262	-1.364647	0.000000	-0.357
	H	0.970272	0.794017	-1.684176	-0.417		H	5.025262	1.364647	0.000000	-0.357
D_1+H	Al	2.392680	-0.177174	0.000345	0.761	D_2+H	H	0.000000	0.000000	0.000000	-0.798
	H	3.173144	0.083746	1.373825	-0.353		Li	-1.683668	0.000000	0.000000	0.826
	H	0.893185	0.581014	-0.001045	-0.502		Li	1.683668	0.000000	0.000000	0.826
	H	3.175694	0.083407	-1.371755	-0.353		Al	-4.273600	0.000000	0.000000	0.659
	H	1.715005	-1.709700	-0.000413	-0.448		Al	4.273600	0.000000	0.000000	0.659
	Li	-0.012144	-1.138196	-0.002474	0.844		H	-3.144215	0.000000	1.224097	-0.434
	H	-2.003764	1.371279	0.000677	-0.407		H	3.144215	0.000000	1.224097	-0.434
	Al	-2.347117	-0.214830	0.000376	0.689		H	-3.144215	0.000000	-1.224097	-0.434
	H	-3.900876	-0.589120	0.000992	-0.343		H	3.144215	0.000000	-1.224097	-0.434
	Li	-0.257440	2.210301	-0.000795	0.758		H	-5.130525	1.363382	0.000000	-0.359
	H	-1.462564	-0.894606	-1.224556	-0.420		H	5.130525	-1.363382	0.000000	-0.359
	H	-1.460897	-0.895695	1.223288	-0.419		H	-5.130525	-1.363382	0.000000	-0.359

	H	0.087503	3.849405	-0.000576	-0.806		H	5.130525	1.363382	0.000000	-0.359
D_1+2H	Al	0.676347	-1.073437	1.685021	0.704	D_2+2H	Li	0.000000	1.726789	0.079428	0.850
	H	1.124808	-1.780372	3.051921	-0.350		Li	0.000000	-1.726789	0.079428	0.850
	H	1.906077	-0.692678	0.662561	-0.408		Al	0.000000	4.272109	-0.024643	0.660
	H	-0.180900	-2.027069	0.656382	-0.408		Al	0.000000	-4.272109	-0.024643	0.660
	H	-0.192034	0.285118	1.970226	-0.442		H	0.000000	3.180371	1.240432	-0.445
	Li	-0.966136	1.513936	0.872261	0.781		H	0.000000	-3.180371	1.240432	-0.445
	H	0.192034	-0.285118	-1.970226	-0.442		H	0.000000	3.082077	-1.197601	-0.445
	Al	-0.676347	1.073437	-1.685021	0.704		H	0.000000	-3.082077	-1.197601	-0.445
	H	-1.124808	1.780372	-3.051921	-0.350		H	1.362626	5.125694	-0.058280	-0.359
	Li	0.966136	-1.513936	-0.872261	0.781		H	-1.362626	-5.125694	-0.058280	-0.359
	H	-1.906077	0.692678	-0.662561	-0.408		H	-1.362626	5.125694	-0.058280	-0.359
	H	0.180900	2.027069	-0.656382	-0.408		H	1.362626	-5.125694	-0.058280	-0.359
	H	-1.807551	2.842157	1.830832	-0.377		H	-0.505331	0.000000	0.155808	-0.401
	H	1.807551	-2.842157	-1.830832	-0.377		H	0.505331	0.000000	0.155808	-0.401
T1	Al	0.992576	3.004913	-0.011258	0.618						
	H	1.469432	4.536488	-0.020267	-0.353						
	H	1.581352	2.065856	-1.225691	-0.406						
	H	1.536633	2.094545	1.246881	-0.406						
	H	-0.654634	2.907133	-0.033991	-0.460						
	Li	-0.379800	-1.735055	-0.034222	0.669						
	H	2.834412	-0.882261	0.043547	-0.461						
	Al	2.108577	-2.363431	0.002266	0.621						
	H	3.205014	-3.533671	-0.007747	-0.352						
	Li	1.709970	0.545041	0.024560	0.673						
	H	1.002965	-2.423201	1.218715	-0.405						
	H	1.042873	-2.366890	-1.251508	-0.407						
	H	-4.662042	-1.010862	-0.013841	-0.352						
	Al	-3.099784	-0.647899	-0.006401	0.619						
	H	-2.179548	-2.015275	-0.067632	-0.460						
	Li	-1.334671	1.219250	0.087629	0.677						
	H	-2.584480	0.253335	1.272782	-0.408						
	H	-2.596267	0.370516	-1.195048	-0.405						
T_2	Al	-0.335147	4.182838	0.000000	0.581	T_3	Li	0.926783	1.630477	0.002064	0.609
	H	-0.587093	5.753403	0.000000	-0.326		Li	0.940471	-1.622508	-0.007022	0.608
	H	-1.606892	3.129673	0.000000	-0.404		Li	-1.881700	-0.008354	-0.003167	0.607
	H	0.493510	3.466567	1.232851	-0.400		Al	2.192691	3.815879	0.000283	0.680
	H	0.493510	3.466567	-1.232851	-0.400		Al	2.217253	-3.801744	0.000771	0.680
	Li	0.000000	1.885181	0.000000	0.617		Al	-4.407149	-0.014055	0.000553	0.680

	H	-1.906930	-2.956446	0.000000	-0.404		H	1.963539	4.907336	-1.151512	-0.349
	Al	-3.454871	-2.381665	0.000000	0.581		H	3.288882	-4.140523	-1.142502	-0.349
	H	-4.689047	-3.385139	0.000000	-0.326		H	-5.237972	-0.710411	-1.180571	-0.349
	Li	-1.632615	-0.942591	0.000000	0.617		H	3.254580	4.163097	1.150028	-0.349
	H	-3.248890	-1.305891	-1.232851	-0.400		H	1.986269	-4.896815	1.148689	-0.349
	H	-3.248890	-1.305891	1.232851	-0.400		H	-5.238224	0.678060	1.183979	-0.349
	H	3.513822	-0.173227	0.000000	-0.404		H	0.732574	3.318694	0.661021	-0.461
	Al	3.790017	-1.801174	0.000000	0.581		H	2.499660	-2.286417	0.663988	-0.461
	H	5.276139	-2.368264	0.000000	-0.326		H	-3.241206	-1.053771	0.613228	-0.462
	Li	1.632615	-0.942591	0.000000	0.617		H	2.487719	2.300913	-0.658255	-0.462
	H	2.755380	-2.160675	-1.232851	-0.400		H	0.759083	-3.311166	-0.669154	-0.461
	H	2.755380	-2.160675	1.232851	-0.400		H	-3.247907	1.031116	-0.615459	-0.462
T_{12}+H	Al	-2.648703	-1.805244	0.000000	0.680	T_3+H	Li	-0.849887	1.553867	-0.004538	0.837
	H	-3.947045	-2.743661	0.000000	-0.348		Li	-0.913654	-1.517825	0.002670	0.837
	H	-1.253802	-2.683084	0.000000	-0.437		Li	1.780558	-0.036495	-0.001562	0.837
	H	-2.544359	-0.729878	1.238979	-0.401		Al	-2.083132	3.763986	0.000386	0.689
	H	-2.544359	-0.729878	-1.238979	-0.401		Al	-2.231197	-3.678670	0.000099	0.689
	Li	-1.638722	0.581115	0.000000	0.837		Al	4.310605	-0.085179	0.000307	0.689
	H	2.951276	0.254905	0.000000	-0.437		H	-1.800539	4.872307	1.124289	-0.350
	Al	2.887701	-1.391612	0.000000	0.680		H	-3.341030	-3.979719	1.117658	-0.350
	H	4.349318	-2.047450	0.000000	-0.348		H	5.127662	-0.827786	1.163189	-0.350
	Li	0.316361	-1.708822	0.000000	0.837		H	-3.176947	4.110210	-1.119854	-0.350
	H	1.904483	-1.838344	-1.239015	-0.401		H	-1.988009	-4.800188	-1.119954	-0.350
	H	1.904483	-1.838344	1.239015	-0.401		H	5.158425	0.624599	-1.161031	-0.350
	H	-1.696490	2.427873	0.000000	-0.437		H	-0.653694	3.237158	-0.700558	-0.450
	Al	-0.239077	3.196514	0.000000	0.680		H	-2.472539	-2.174635	-0.701100	-0.450
	H	-0.402220	4.790142	0.000000	-0.348		H	3.133448	-1.089748	-0.645619	-0.450
	Li	1.322555	1.128961	0.000000	0.837		H	-2.384323	2.268439	0.696507	-0.450
	H	0.639577	2.568934	-1.238940	-0.401		H	-0.784860	-3.205273	0.704345	-0.450
	H	0.639577	2.568934	1.238940	-0.401		H	3.172584	0.964620	0.644336	-0.450
	H	0.000000	0.000545	0.000000	-0.786		H	0.007195	-0.000410	-0.002211	-0.776
T_{12}+2H	Al	-2.611791	1.948512	0.000000	0.686	T_3+2H	Li	0.000000	1.800351	0.000000	0.856
	H	-3.958929	2.811750	0.000000	-0.343		Li	-1.560319	-0.901741	0.000000	0.856
	H	-2.909657	0.325131	0.000000	-0.442		Li	1.561861	-0.900957	0.000000	0.856
	H	-1.572658	2.227724	1.238864	-0.394		Al	-3.140732	1.811774	0.000000	0.774
	H	-1.572658	2.227724	-1.238864	-0.394		Al	-0.000145	-3.626113	0.000000	0.775
	Li	0.000000	1.752901	0.000000	0.856		Al	3.140621	1.814970	0.000000	0.775
	H	1.173256	-2.682402	0.000000	-0.442		H	-3.870568	2.233406	1.367100	-0.361
	Al	-0.381565	-3.236134	0.000000	0.686		H	0.000177	-4.469614	1.366710	-0.361

	H	-0.455582	-4.834408	0.000000	-0.343		H	3.870651	2.236282	1.367001	-0.361
	Li	-1.518057	-0.876451	0.000000	0.856		H	-3.870568	2.233406	-1.367100	-0.361
	H	-1.142937	-2.475824	-1.238864	-0.394		H	0.000177	-4.469614	-1.366710	-0.361
	H	-1.142937	-2.475824	1.238864	-0.394		H	3.870651	2.236282	-1.367001	-0.361
	H	1.736400	2.357271	0.000000	-0.442		H	-1.609185	2.436516	0.000000	-0.486
	Al	2.993357	1.287622	0.000000	0.686		H	-1.307070	-2.612638	0.000000	-0.486
	H	4.414511	2.022658	0.000000	-0.343		H	2.916992	0.175957	0.000000	-0.486
	Li	1.518057	-0.876451	0.000000	0.856		H	-2.917829	0.172583	0.000000	-0.486
	H	2.715595	0.248100	-1.238864	-0.394		H	1.306435	-2.611734	0.000000	-0.486
	H	2.715595	0.248100	1.238864	-0.394		H	1.608656	2.439371	0.000000	-0.486
	H	0.000000	0.000000	0.707006	-0.452		H	0.000091	-0.000681	-0.527108	-0.407
	H	0.000000	0.000000	-0.707006	-0.452		H	0.000091	-0.000681	0.527108	-0.407

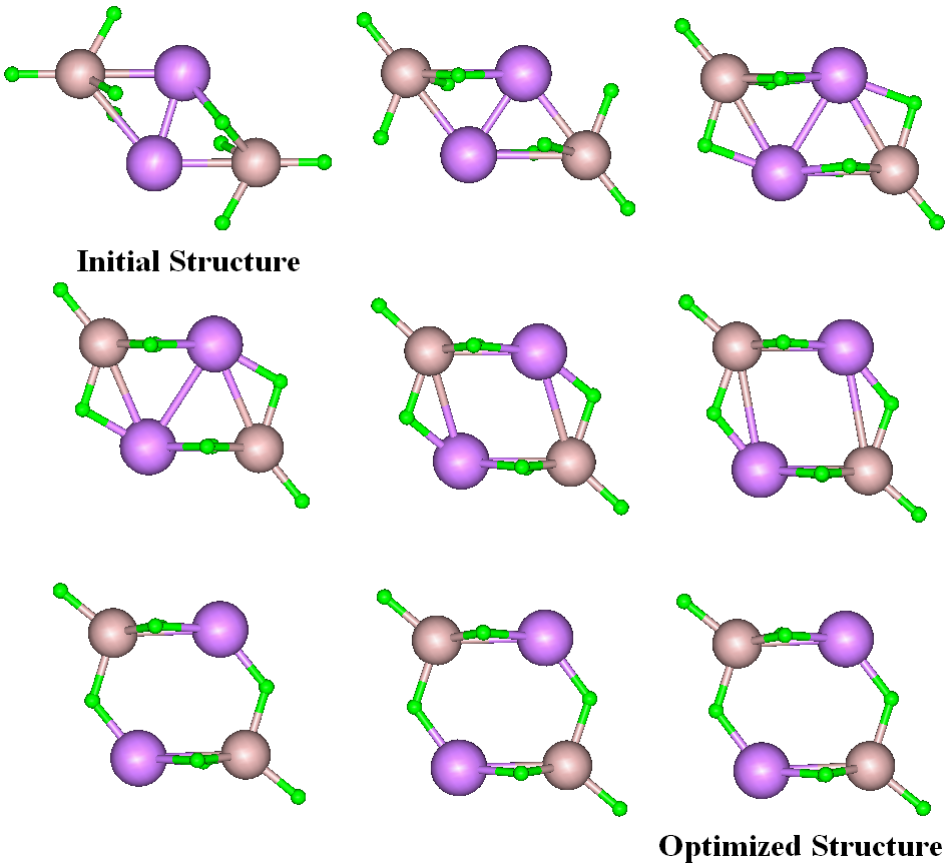
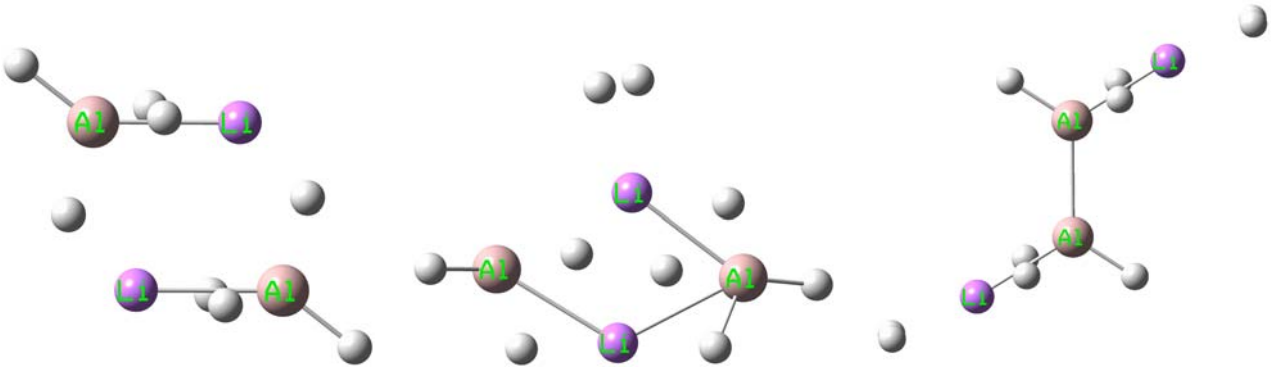


Figure S1. The reorganization process of $\mathbf{D_1}$.



Neutral Dimer **Hydrogenated Dimer** **Dihydrogenated Dimer**

Figure S2. The optimized structures of neutral dimer and the hydrogenated dimers.

Complete Ref. 17:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.;Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. GAUSSIAN 03, Revision C.02, Gaussian, Inc., Wallingford CT, 2004.