Supplementary Information

A Ligand-Induced Homojunction between Aluminum-based Superatomic Clusters

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Supplementary Table 1. Energies of HOMO and LUMO levels, adiabatic ionization energy, and HOMO-LUMO gap (in eV). The gross charge on Al_{13} and PAl_{12} in Al_{13}(EP) and PAl_{12}(EP) are given by the Hirshfeld charge analysis.

Cluster	HOMO (eV)	LUMO (eV)	AIE (eV)	HL gap	Hirshfeld Charges (e^-)	Dipole Moment (Debye)
Al_{13}	-5.108	-4.700	6.13	0.408		
PAl_{12}	-3.724	-3.156	5.10	0.568		
Al_{13}(EP)	-4.407	-3.697	5.08	0.710	-0.369	14.16
PAl_{12}(EP)	-3.134	-2.517	4.36	0.617	-0.349	13.91

$PAl_{12}(Ge^{1}_{B})$			$CH_3CH_3GeCH_3CH_3$		
1	P	-0.1325	1	H	0.0334
2	Al	0.0227	2	H	0.0333
3	Al	0.0193	3	H	0.0337
4	**Al**	***0.1342***	4	H	0.0335
5	Al	0.0205	5	H	0.0336
6	Al	0.0276	6	H	0.0336
7	Al	0.0197	7	H	0.0335
8	Al	0.0200	8	H	0.0334
9	Al	-0.0247	9	H	0.0335
10	Al	0.0196	10	H	0.0336
11	Al	0.0241	11	H	0.0336
12	Al	0.0190	12	H	0.0337
13	Al	0.0182	13	C	-0.1961
14	H	0.0332	14	C	-0.1964
15	H	0.0335	15	C	-0.1963
16	H	0.0205	16	C	-0.1960
17	H	0.0234	17	Ge	0.3825
18	H	0.0234	**Charges in bold-italic text are for the atoms in Al-C connecting bond in $PAl_{12}[Ge^{1}_{B}]$.**		
19	H	0.0334			
20	H	0.0197			
21	H	0.0331			
22	H	0.0325			
23	H	0.0324			
24	H	0.0322			
25	C	-0.1973			
26	C	-0.1970			
27	**C**	***-0.2863***			
28	C	-0.1976			
29	Ge	0.3696			

Supplementary Table 2. Hirshfeld Charge Analysis of $PAl_{12}Ge^{1}_{B}$ and Ge-linker ($CH_3CH_3GeCH_3CH_3$).

Supplementary Table 3. Hirshfeld Charge Analysis of $PAl_{12}Ge^{1}_{B}$ and Ge-linker ($CH_3CH_3GeCH_3CH_3$).

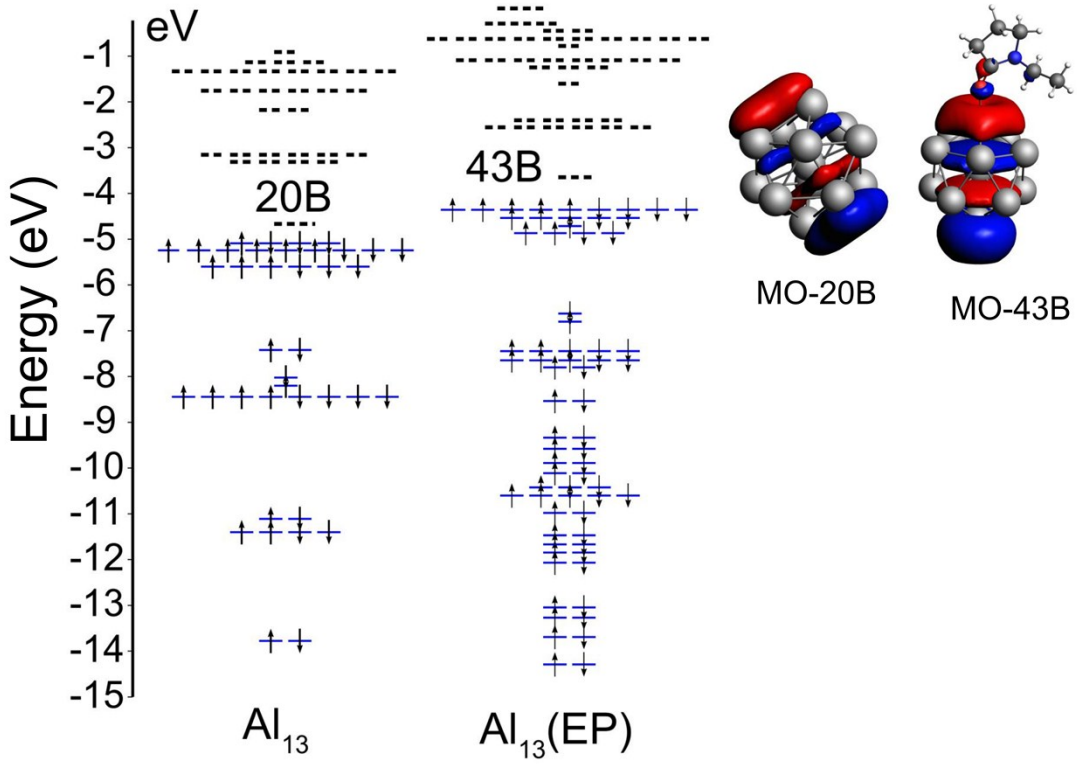
$(EP)_nPAl_{12}Ge^{2}_{B}PAl_{12}$	**Hirshfeld-charge**				
No. of EP (n)	EP	Left-PAl_{12} (ligated)	Net Ligated	Ge^{2}_{B}	Right-PAl_{12} (non-ligated)
0	0	0.184	+0.1836	-0.367	0.181
1	0.346	-0.12	+0.2300	-0.399	0.168
2	0.615	-0.359	+0.2554	-0.407	0.147
3	0.825	-0.537	+0.288	-0.418	0.129
4	0.947	-0.632	+0.315	-0.431	0.124

Supplementary Table 4. The HOMO, LUMO, and HOMO-LUMO Gap of $(EP)_nPAl_{12}[Ge^{1}_{B}]$, n=0-4.

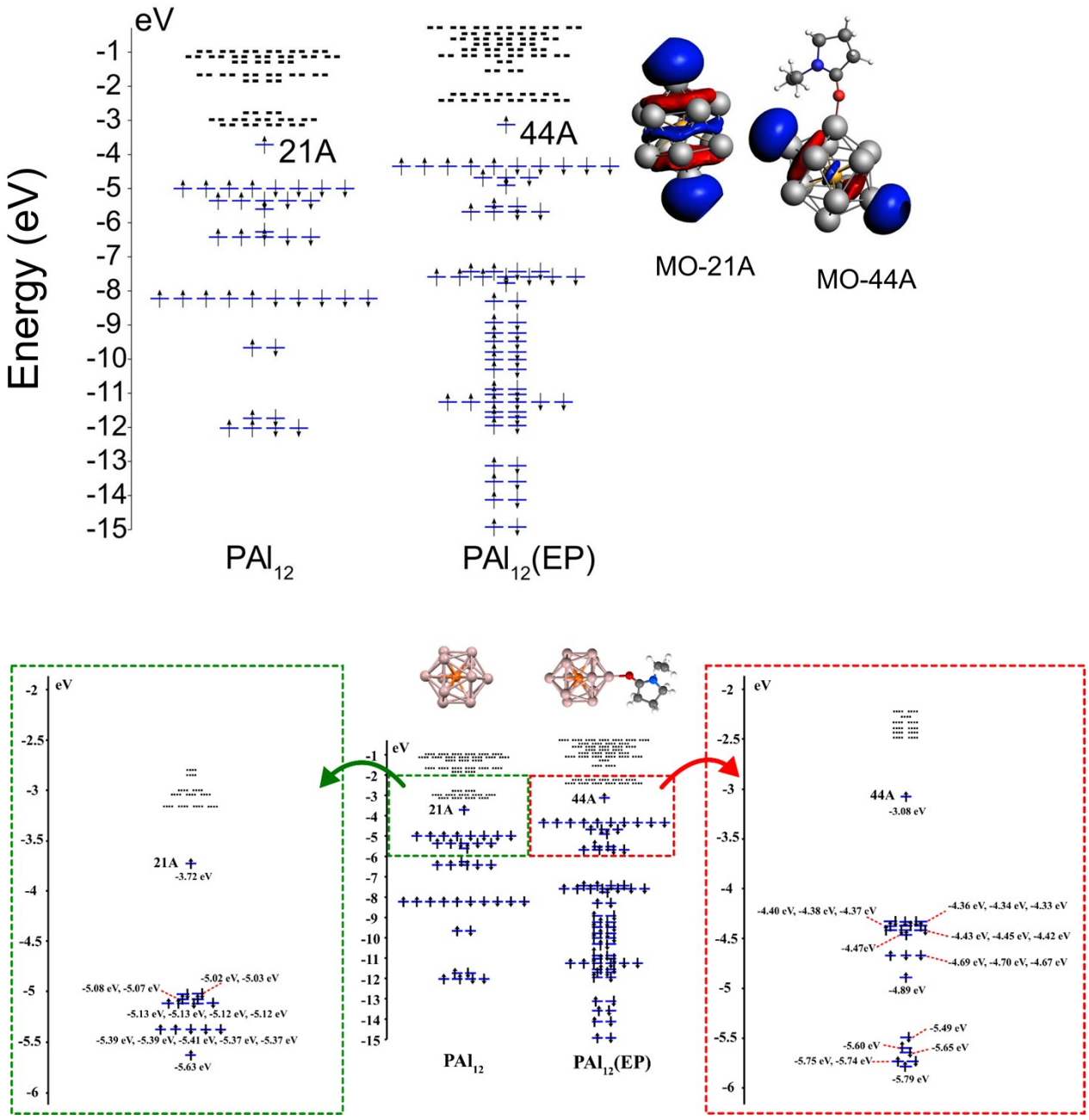
$(EP)_nPAl_{12}[Ge^{1}_{B}]$	HOMO (eV)	LUMO (eV)	GAP (eV)
0	-4.775	-3.13	1.645
1	-4.15	-2.526	1.624
2	-3.597	-1.986	1.611
3	-3.098	-1.65	1.448
4	-2.811	-1.43	1.381

Supplementary Table 5. The 4 lowest energy absorption processes are shown for $(EP)PAl_{12}Ge^{2}_{B}PAl_{12}$. The 79a is the HOMO, and 80a

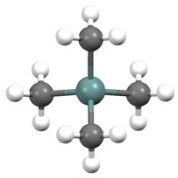
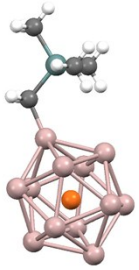
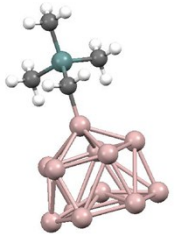
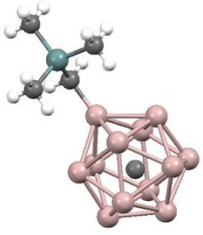
Transitions			Weight (sum=1)	contributions to transition dipole moment			E/eV	Oscillator strengths (f)
				x	y	z		
HOMO	->	80a	0.9998	0.0051	0.0155	-0.0179	1.12694	6.953E-07
79a	->	81a	0.9998	0.0105	-0.0069	0.0061	1.13039	4.057E-07
79a	->	82a	0.9879	0.0564	0.2081	0.1706	1.24892	0.0006201
79a	->	83a	0.9879	0.2267	-0.031	-0.1127	1.25286	0.0005652



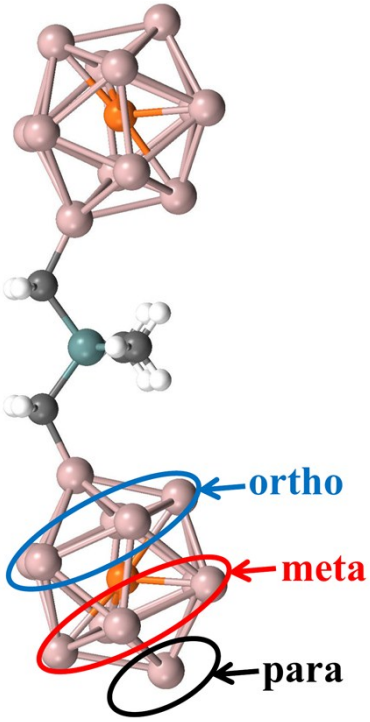
Supplementary Figure 1. One-electron energy levels of Al_{13} and Al_{13}(EP). Molecular orbital surfaces of LUMO in Al_{13} and Al_{13}(EP) are shown.



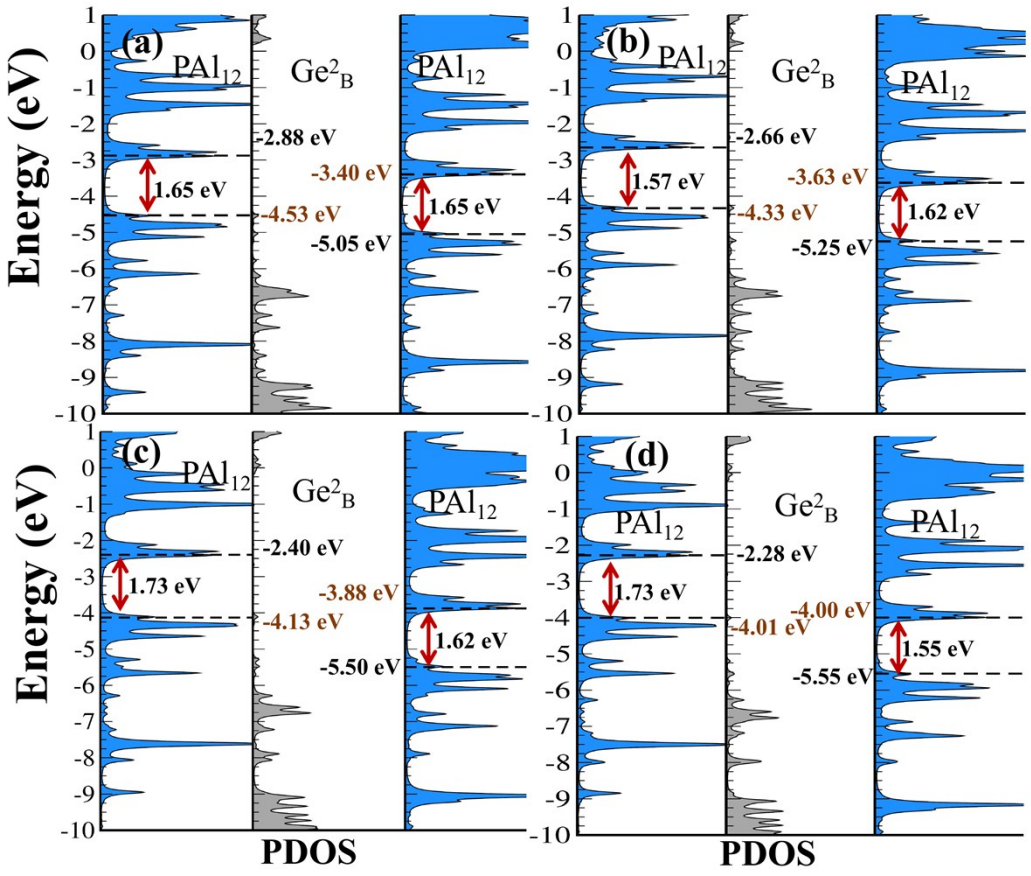
Supplementary Figure 2. One-electron energy levels of PAl_{12} and PAl_{12}(EP). Molecular orbital surfaces of HOMO in PAl_{12} and PAl_{12}(EP) are shown. A blown up version of the levels is shown below.

			
$Ge\{(CH_3)_2\}_2$; M = 0 μ_B HL- Gap = 6.23 eV Dipole = 0.00 D AIP = 8.75 eV AEA = -0.99 eV	**$PAl_{12}Ge^1_B$;** M = 0 μ_B HL Gap = 1.65 eV Dipole = 0.58 D AIP = 6.13 eV AEA = 1.88 eV	**$Al_{13}Ge^1_B$;** M = 0 μ_B HL Gap= 1.45 eV Dipole= 0.20 D AIP= 6.34 eV AEA= 2.00 eV	**$CAl_{12}Ge^1_B$** ; M = 1 μ_B HL-Gap = 0.51 eV; Dipole = 0.86 D; AIP = 5.96 eV AEA =2.81 eV

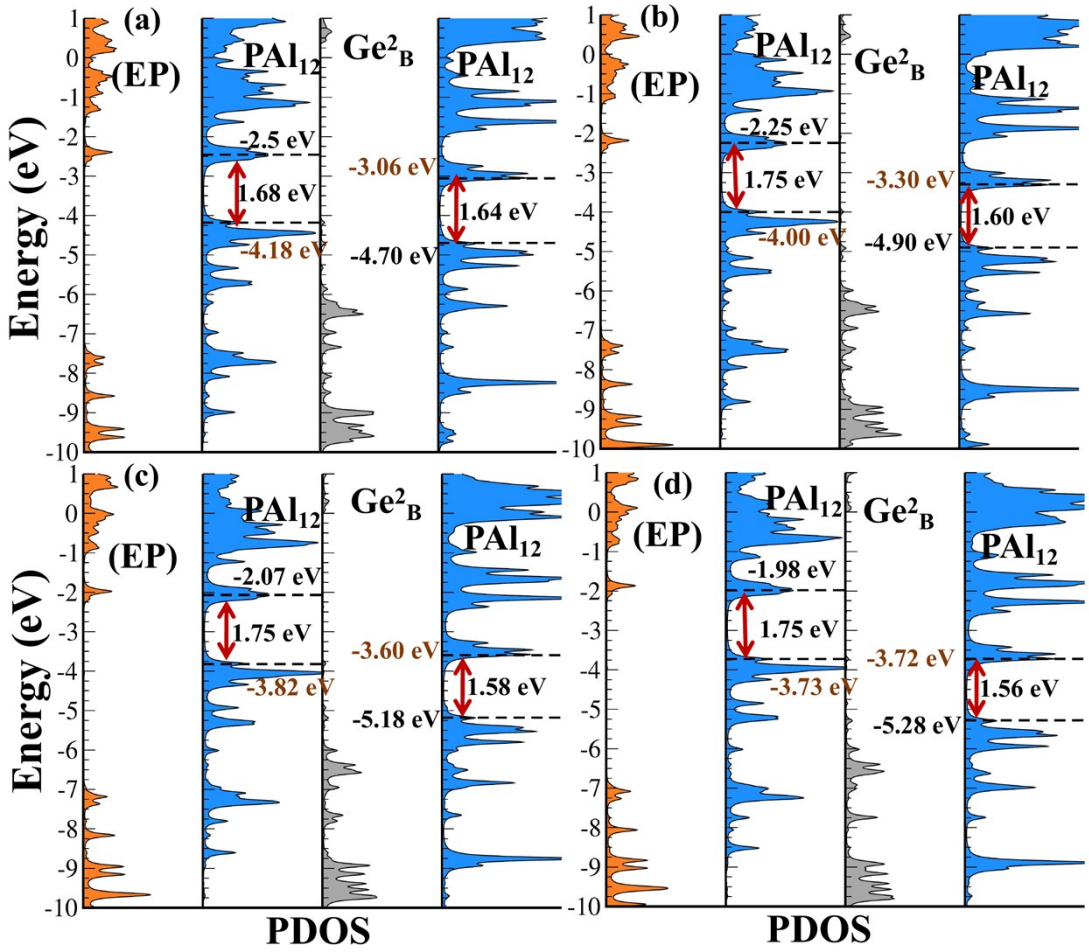
Supplementary Figure 3. Optimized ground state structure of tetramethyl germane $CH_3CH_3GeCH_3CH_3$ (=Ge-linker), $PAl_{12}Ge^1_B$, $Al_{13}Ge^1_B$, and $CAl_{12}Ge^1_B$ respectively. Their electronic properties, total magnetic moment (in μ_B), and dipole moments in Debye(D) are also given.



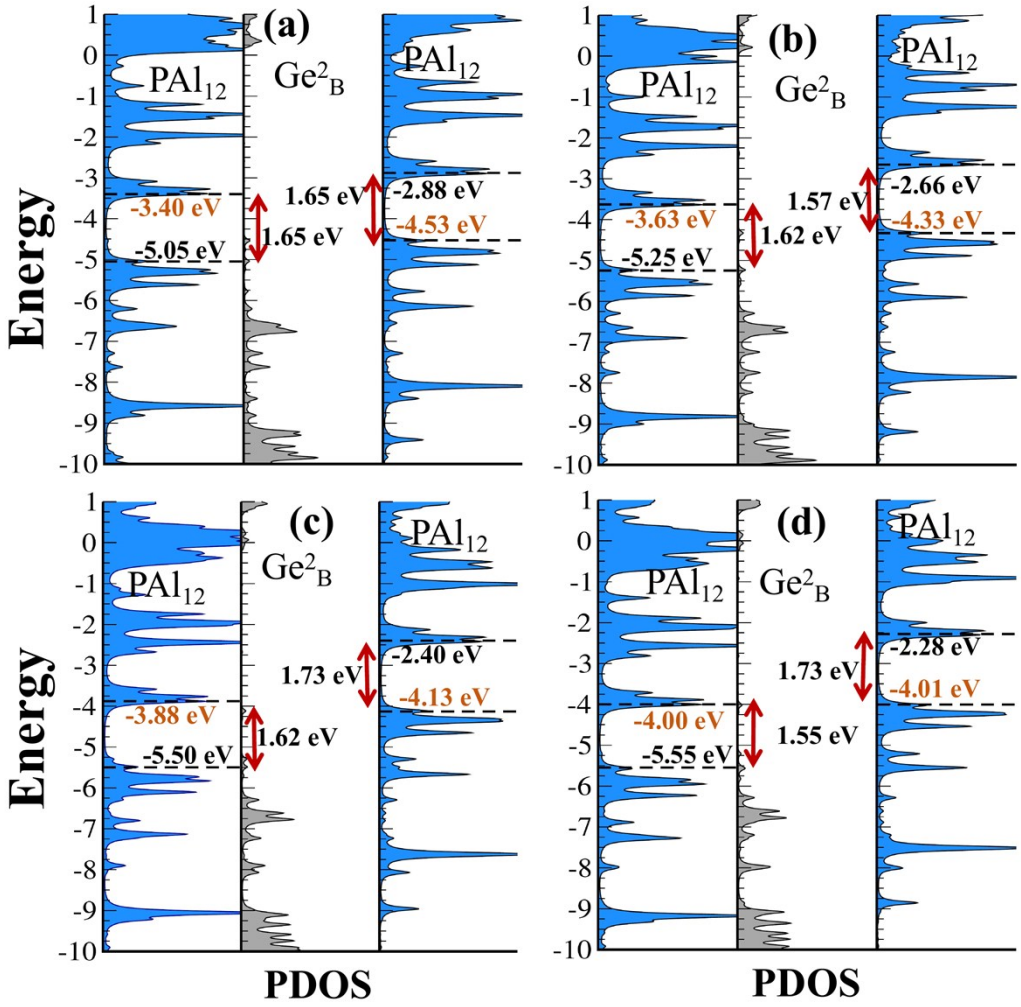
Supplementary Figure 4. Depiction of *Ortho*-, *Meta*-, and *Para*-Al sites for attaching EP (= $C_6H_{11}NO$) ligand in $PAl_{12}Ge^2{}_BPAl_{12}$.



Supplementary Figure 5. Partial density of states for $PAl_{12}[Ge^2_B]PAl_{12}$ molecule in the presence of applied homogenous electric fields: **(a)** -0.001 a.u. , **(b)** -0.002 a.u. , **(c)** -0.003 a.u., and **(d)** -0.0036 a.u.



Supplementary Figure 6. Partial density of states for (EP)$PAl_{12}[Ge^2_B]PAl_{12}$ molecule in the presence of applied homogenous electric fields: (**a**) -0.000 a.u. , (**b**) -0.001 a.u., (**c**) -0.002 a.u., and (**d**) -0.0026 a.u.



Supplementary Figure 7. Partial density of states for $PAl_{12}[Ge^2_B]PAl_{12}$ molecule in the presence of applied homogenous electric fields: (**a**) 0.001 a.u., (**b**) 0.002 a.u., (**c**) 0.003 a.u., and (**d**) 0.0036 a.u.

Cartesian co-ordinates of optimized ground state structures of $(EP)_nPAl_{12}Ge^2_BPAl_{12}$, for n= 0, 1, 2, 3, and respectively.

$PAl_{12}Ge^2_BPAl_{12}$

41
XYZ
P -0.043747 0.292629 -6.228118
Al -2.201637 0.199426 -4.675824
Al -1.581587 2.377416 -6.342846
Al 0.065293 -1.01401 -3.476046
Al -1.231905 -2.048675 -5.789868
Al -0.122933 1.776992 -4.026275
Al -2.293853 -0.066465 -7.469431
Al 1.199779 2.560266 -6.370641
Al -0.148297 1.462896 -8.681599
Al 1.448348 -1.871577 -5.818045
Al 2.135598 0.486291 -4.717151
Al 0.0484 -1.38302 -8.204109
Al 2.204139 0.232578 -7.512329
Al -1.159481 -2.23582 5.672729
Al 1.518059 -2.031043 5.672877
Al 0.100445 -1.102459 3.379542
Al 0.142279 -1.642087 8.090886
Al -2.163178 0.040659 4.649532
Al 2.170462 0.370353 4.650553
P 0.010186 0.101407 6.178327
Al -2.219948 -0.322926 7.432874
Al 2.275007 0.016595 7.432374
Al -0.10827 1.664664 4.032379
Al -0.074207 1.182806 8.673498
Al -1.544797 2.164711 6.385833
Al 1.23538 2.374463 6.388298
H -2.517518 -0.427149 -0.034114
C -1.677058 0.277377 -0.021449
H -0.662609 -2.670613 1.504259
H -1.741922 0.89212 0.884915
H -1.744084 0.927205 -0.902755
H -0.653273 -2.63966 -1.631371
C 0.168118 -1.952085 1.593069
Ge 0.070661 -0.746282 -0.042486
C 0.164765 -1.905512 -1.711294
H 1.102972 -2.528913 1.505163
H 1.109065 -2.470431 -1.649614
C 1.629167 0.546922 -0.025941
H 1.596287 1.163959 0.880612
H 1.588455 1.198807 -0.907308
H 2.572789 -0.011979 -0.040915

$(EP)PAl_{12}Ge^2_BPAl_{12}$

60
XYZ
P 0.5245 1.538 -5.37507
Al -1.35569 1.15659 -3.54
Al -1.04413 3.53517 -5.03134
Al 1.02013 -0.08812 -2.80903
Al -0.67027 -1.01125 -4.96505
Al 0.76167 2.7451 -3.06002
Al -1.88926 1.17961 -6.24448
Al 1.7577 3.86859 -5.51717
Al 0.02624 2.84941 -7.64387
Al 1.9553 -0.70622 -5.34941
Al 2.86852 1.54936 -4.20737
Al 0.26952 -0.03943 -7.42243
Al 2.52697 1.52321 -6.97658
Al -0.61908 -2.4123 5.86302
Al 1.92793 -1.79931 6.44694
Al 0.8522 -0.85098 3.97406
Al 0.05502 -1.89895 8.54447
Al -1.78162 -0.22015 4.82853
Al 2.33447 0.7723 5.77436
P 0. 0. 6.78593
Al -2.32142 -0.89626 7.49955
Al 1.95464 0.13223 8.4827
Al 0.03718 1.75867 4.7897
Al -0.75948 0.77495 9.2815
Al -1.90033 1.76694 6.81351
Al 0.74495 2.39983 7.42336

H -1.49847 -0.2648 0.59047
C -0.78365 0.5638 0.67669
H 0.8126 -2.37033 1.9205
H -0.96325 1.08951 1.62212
H -0.94091 1.25672 -0.15923
H 0.75402 -2.01867 -1.11753
C 1.38247 -1.45997 2.16823
Ge 1.11109 -0.15821 0.61778
C 1.39448 -1.1216 -1.14703
H 2.44862 -1.73754 2.16751
H 2.4389 -1.47239 -1.16
C 2.42262 1.37082 0.8183
H 2.24593 1.89427 1.76664
H 2.30519 2.07827 -0.01106
H 3.44879 0.98231 0.81144
H -1.33147 -5.67296 -6.79346
C -1.76052 -6.32204 -6.01905
H -2.6652 -6.79748 -6.42012
H -1.0351 -7.11584 -5.79827
H -5.11666 -3.33001 -6.61224
H -4.67114 -5.50383 -5.74906
C -2.04989 -5.52742 -4.74763
H -3.77546 -1.49074 -5.80449
O -1.51141 -2.7398 -4.82426
N -3.01543 -4.45098 -4.95563
C -2.70053 -3.15151 -4.95425
C -5.01641 -3.32913 -5.5192
C -4.46163 -4.6868 -5.04675
H -1.13352 -5.05801 -4.36883
C -3.94363 -2.31339 -5.09474
H -2.44741 -6.18286 -3.95774
H -6.00184 -3.11876 -5.09105
H -4.84588 -4.98071 -4.05538
H -4.14826 -1.84365 -4.11893

$(EP)_2PAl_{12}Ge^2_BPAl_{12}$

79
XYZ
P -0.30793 1.01073 -5.2215
Al -2.29994 1.04636 -3.52505
Al -1.52272 3.23899 -5.09541
Al -0.17476 -0.44869 -2.51503
Al -1.80486 -1.28046 -4.73506
Al 0.02227 2.29116 -2.96004
Al -2.70688 0.95945 -6.32794
Al 1.30579 3.10304 -5.34755
Al -0.37821 2.20692 -7.56603
Al 0.8704 -1.35096 -4.87768
Al 2.0666 0.79328 -3.80154

Al -0.56466 -0.6745 -7.14333
Al 1.83783 0.61131 -6.56664
Al -1.16552 -2.31516 6.63808
Al 1.50198 -2.07253 6.51937
Al -0.03801 -1.01819 4.35044
Al 0.24944 -1.85725 9.02841
Al -2.24441 0.00403 5.81459
Al 2.06959 0.39987 5.62413
P 0.000 0.000 7.24151
Al -2.15907 -0.53899 8.57023
Al 2.32573 -0.12845 8.37057
Al -0.24981 1.69629 5.20578
Al 0.02739 0.92004 9.80139
Al -1.5711 2.02064 7.65433
Al 1.20044 2.27517 7.53596
H -2.56265 0.22434 1.11683
C -1.63656 0.81249 1.09703
H -0.97941 -2.35365 2.39043
H -1.57397 1.40681 2.01783
H -1.66221 1.4854 0.23124
H -1.00892 -2.10985 -0.72765
C -0.07152 -1.74165 2.51595
Ge -0.04349 -0.42982 0.9459
C -0.11602 -1.46557 -0.78963
H 0.78891 -2.41573 2.37607
H 0.75898 -2.13604 -0.79395
C 1.66918 0.65639 1.03634
H 1.68541 1.27095 1.94515
H 1.73216 1.3066 0.15407
H 2.53155 -0.02234 1.04567
H -2.97921 -5.86457 -6.30785
C -3.63623 -6.39031 -5.60335
H -4.53634 -6.71741 -6.14192
H -3.11263 -7.28801 -5.24953
H -6.33452 -2.93661 -6.78616
H -6.40303 -5.08676 -5.76509
C -3.9791 -5.49367 -4.41504
H -4.78748 -1.30396 -5.89583
O -2.93083 -2.85835 -4.5637
N -4.69804 -4.28329 -4.80331
C -4.14899 -3.06156 -4.82833
C -6.37072 -2.87336 -5.69047
C -6.13787 -4.26919 -5.08032
H -3.06565 -5.16925 -3.90218
C -5.1908 -2.03411 -5.17762
H -4.60445 -6.0327 -3.68648
H -7.34616 -2.46208 -5.40992
H -6.69306 -4.4191 -4.13911
H -5.42549 -1.46386 -4.26422
H 5.57079 1.56989 1.16347
C 5.57329 2.05869 0.18059
H 4.60277 2.55234 0.04465
H 6.36183 2.82329 0.18766
C 5.80388 1.01462 -0.90977
H 4.99559 0.27217 -0.90624
H 6.75602 0.48481 -0.75154
N 5.83383 1.59247 -2.25086
O 3.7859 0.8231 -2.90107
H 7.3739 3.03039 -2.05125
C 4.85393 1.45226 -3.1509
C 7.0003 2.30481 -2.78498
H 6.14199 3.99579 -3.84573
H 7.80801 1.58165 -2.99125
C 6.45853 2.96822 -4.06592
C 5.23514 2.11876 -4.44495
H 4.38152 2.68402 -4.84865
H 7.2149 3.01168 -4.85647
H 5.45973 1.33052 -5.18219

$(EP)_3PAl_{12}Ge^2{}_BPAl_{12}$

98
XYZ
P -0.06833 0.26195 -5.08497
Al -2.26331 0.488 -3.68549
Al -1.18557 2.53616 -5.19953
Al -0.42983 -0.99608 -2.30281
Al -1.68511 -1.89273 -4.731
Al -0.06318 1.74914 -2.75644
Al -2.25844 0.24573 -6.51746
Al 1.61152 2.32479 -4.97166
Al 0.2955 1.37862 -7.41479
Al 0.96097 -2.04591 -4.39782
Al 1.99045 0.13644 -3.21872

Al -0.02936 -1.51012 -7.00457
Al 2.26598 -0.20535 -5.98005
Al -0.73946 -2.54131 7.09549
Al 1.6937 -1.75679 6.2844
Al -0.51874 -1.21631 4.56427
Al 1.0864 -1.63457 9.0265
Al -2.46951 -0.56964 6.54001
Al 1.47346 0.70841 5.23702
P 0.000 0.000 7.3342
Al 2.50302 0.44405 7.83728
Al -1.10373 1.44138 5.39342
Al 0.45875 1.09065 9.78621
Al -1.82226 1.67707 8.09546
Al 0.7072 2.49315 7.27032
H -2.92905 0.24698 1.22422
C -1.91372 0.65849 1.17133
H -1.88567 -2.38596 2.74163
H -1.74206 1.30563 2.0426
H -1.80998 1.246 0.25168
H -1.73913 -2.36885 -0.53968
C -0.84736 -2.02128 2.79458
Ge -0.55341 -0.84493 1.14113
C -0.72664 -1.93293 -0.54771
H -0.1922 -2.90019 2.67134
H -0.0165 -2.77145 -0.45828
C 1.305 -0.02893 1.25699
H 1.35238 0.68557 2.09029
H 1.5341 0.49226 0.31832
H 2.04674 -0.82008 1.42079
H -2.79027 -6.78815 -3.45612
C -3.88284 -6.89621 -3.4388
H -4.16277 -7.73543 -4.08987
H -4.18449 -7.15232 -2.41492
H -3.1549 -5.91969 -7.82044
H -4.75256 -6.89282 -6.34866
C -4.55943 -5.59433 -3.86321
H -2.3417 -3.69832 -7.3106
O -2.88412 -3.43242 -4.61213
N -4.21138 -5.18614 -5.22002
C -3.4354 -4.12984 -5.50747
C -3.96362 -5.22162 -7.56752
C -4.80496 -5.7978 -6.41332
H -4.25868 -4.77147 -3.20233
C -3.37196 -3.92313 -6.99606
H -5.65566 -5.68967 -3.81048
H -4.56249 -5.06025 -8.46987
H -5.86876 -5.51054 -6.48131
H -3.96116 -3.02308 -7.2371
H 5.50065 -0.04703 2.04992
C 5.67172 0.49909 1.11305
H 4.93104 1.30759 1.05098
H 6.6751 0.94391 1.16321
C 5.5279 -0.45502 -0.06999
H 4.51615 -0.87854 -0.10053
H 6.24417 -1.28729 0.01278
N 5.74373 0.19287 -1.35964
O 3.57262 0.07121 -2.05896
H 7.64953 1.08095 -1.10517
C 4.77704 0.37756 -2.27417
C 7.07673 0.53375 -1.8654
H 6.78022 2.44356 -2.85717
H 7.62604 -0.3941 -2.10352
C 6.77784 1.37728 -3.11879
C 5.36441 0.94459 -3.53763
H 4.72622 1.74434 -3.93935
H 7.52589 1.22372 -3.90471
H 5.35563 0.14543 -4.29818
H -2.04562 6.43364 -2.98285
H 0.50091 6.11653 -3.51719
H -2.98236 3.67693 -1.74285
C 0.70165 5.60205 -2.56609
H 1.13126 4.62275 -2.82135
C -1.67228 6.34252 -1.94916
N -0.58694 5.35728 -1.92191
C -0.96708 4.17812 -1.41416
H -3.74572 5.97602 -1.32233
C -2.41044 4.24633 -0.98784
O -0.23516 3.14808 -1.36923
C -2.72583 5.74848 -0.99582
H -1.30596 7.32778 -1.62947
C 1.65545 6.41346 -1.692
H 2.597 6.57737 -2.23362
H -2.564 3.74627 -0.02396
H 1.24181 7.39868 -1.43422
H -2.59186 6.16555 0.01158
H 1.8836 5.87774 -0.76216
Al -1.58198 -0.86896 9.19234

$(EP)_4PAl_{12}Ge^2{}_BPAl_{12}$

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XYZ

P	0.07604	0.16039	-3.80904
Al	-1.96791	0.27727	-2.26234
Al	-1.25411	2.39489	-3.91826
Al	0.18646	-1.13003	-1.18241
Al	-1.34599	-2.0973	-3.35102
Al	0.25937	1.69233	-1.62553
Al	-2.31149	0.02576	-5.01005
Al	1.55624	2.30134	-4.06774
Al	-0.05689	1.26037	-6.23302
Al	1.36376	-2.25854	-3.48509
Al	2.34249	0.08808	-2.42905
Al	-0.18294	-1.58828	-5.7637
Al	2.16225	-0.21701	-5.19101
Al	-0.76608	-2.53036	8.15816
Al	1.81945	-1.86424	7.91887
Al	0.1042	-1.3528	5.68976
Al	0.57814	-1.55683	10.43202
Al	-2.2284	-0.54088	7.09864
Al	1.95328	0.54031	6.72834
P	0.000	0.000	8.44746
Al	-2.02017	-0.71804	9.89726
Al	2.33047	0.39722	9.50794
Al	-0.55125	1.36973	6.22693
Al	-0.0956	1.21582	10.87924
Al	-1.88181	1.76923	8.66226
Al	0.8065	2.46413	8.43082
H	-2.44012	-0.58262	2.35348
C	-1.57445	0.09139	2.33459
H	-0.66975	-2.91785	3.81803
H	-1.60342	0.72956	3.22837
H	-1.62766	0.71827	1.43537
H	-0.60596	-2.80192	0.6324
C	0.1796	-2.22373	3.92624
Ge	0.13789	-0.99294	2.28267
C	0.23337	-2.08715	0.59163
H	1.10014	-2.82379	3.84769
H	1.16004	-2.68067	0.64782
C	1.71897	0.27714	2.38959
H	1.64484	0.91014	3.28365
H	1.71883	0.90808	1.49161
H	2.6529	-0.29805	2.42966
H	-3.12818	-6.89258	-4.48553
C	-3.66193	-7.25742	-3.59812
H	-4.67243	-7.5628	-3.89898
H	-3.13944	-8.14865	-3.22605
H	-6.22334	-3.6586	-4.7294
H	-6.27835	-5.70141	-3.50568
C	-3.68993	-6.18605	-2.51038
H	-4.44784	-2.07571	-4.24159
O	-2.50666	-3.67158	-3.09265
N	-4.37998	-4.96918	-2.92262
C	-3.75866	-3.79657	-3.14376
C	-6.07664	-3.50162	-3.65317
C	-5.83998	-4.85624	-2.95839
H	-2.67058	-5.88971	-2.23472
C	-4.77558	-2.72129	-3.41225
H	-4.18999	-6.56528	-1.6045
H	-6.96424	-2.99201	-3.26347
H	-6.23588	-4.87678	-1.92817
H	-4.81199	-2.06652	-2.52577
H	3.44029	3.36279	1.82151
C	3.75361	3.40383	0.76969
H	2.86803	3.24286	0.14039
H	4.15103	4.40936	0.57319
C	4.79669	2.31906	0.5063
H	4.36979	1.32902	0.70888
H	5.67903	2.45271	1.15133
N	5.25379	2.30237	-0.87936
O	4.07449	0.4444	-1.52167
H	5.94601	4.28699	-1.09193
C	4.8735	1.38686	-1.78192
C	6.21252	3.2708	-1.41443
H	5.3863	3.80312	-3.35184
H	7.22116	3.04585	-1.02756
C	6.10288	3.07987	-2.94017
C	5.53842	1.6608	-3.10528
H	4.79534	1.55614	-3.91073
H	7.06488	3.22728	-3.44282
H	6.31527	0.89636	-3.26769
H	3.29598	-1.8565	-9.45201
H	1.20682	-0.32998	-9.84791
H	2.56209	-3.56131	-6.85495
C	0.49745	-1.15139	-9.6701

H -0.168 -0.82448 -8.85988
C 2.57452 -2.65008 -9.70742
N 1.26131 -2.29083 -9.16788
C 0.94227 -2.98293 -8.06395
H 3.97354 -4.0821 -8.80097
C 2.03768 -3.96495 -7.7411
O -0.09021 -2.77663 -7.36678
C 2.90224 -3.98563 -9.00944
H 2.53262 -2.73615 -10.80152
C -0.2916 -1.48103 -10.93512
H -0.83478 -0.58865 -11.27142
H 1.62447 -4.93767 -7.45167
H 0.36262 -1.80712 -11.75616
H 2.60745 -4.82376 -9.65418
H -1.02631 -2.27386 -10.73884
H -4.05324 8.00544 -5.30966
H -5.40027 6.87912 -5.56603
C -4.33243 6.94306 -5.31808
H -3.76593 6.43908 -6.11229
H -2.28707 8.41526 -3.57181
C -4.07491 6.27552 -3.96842
C -2.07284 7.52768 -2.96275
H -4.6763 6.75062 -3.17805
H -0.067 7.58855 -3.79528
H -2.50329 7.69174 -1.95984
N -2.67594 6.33393 -3.56063
C -0.57271 7.18176 -2.90909
H -4.34483 5.21254 -4.00738
H -0.08839 7.6053 -2.02234
C -1.86047 5.26524 -3.53786
C -0.53145 5.64592 -2.94401
O -2.22234 4.12789 -3.93745
H 0.29161 5.21063 -3.5298
H -0.46387 5.17501 -1.94802