Supporting information materials for

Can an Electron-Shell Closing Model Explain the Structure and Stability of Ligand-Stabilized Metal Clusters?

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Complete reference 14

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Absolute energies for aluminum, aluminum hydride and aluminum iodide clusters

	Isomer	Absolute energy (Hartrees)	Relative energy (eV)
Al_7^-		−1696.25927864	
Al_{13}^-		−3150.34560338	
Al_7H	**1o**	−1696.79689595	0.00
	1b	−1696.76319698	0.92
$Al_{13}H$	**1f**	−3150.82696146	0.00
	1o	−3150.81666042	0.28
$Al_{13}H_3$	**2o1b**	−3152.01510096	0.00
	1o2b	−3151.98704731	0.76
Al_7I	**1o**	−1991.97930807	0.00
	1b	−1991.95790161	0.58
$Al_{13}I$	**1b**	−3445.99435467	0.00
	1o	−3445.98602299	0.23

Cartesian coordinates

- Al_7^-

Al	0.288837000	0.934562000	1.365342000
Al	0.288837000	-1.696648000	1.349432000
Al	0.288837000	-1.696648000	-1.349432000
Al	0.288837000	0.934562000	-1.365342000
Al	2.168206000	-0.306047000	0.000000000
Al	-1.613869000	-0.475257000	0.000000000
Al	-1.709686000	2.305475000	0.000000000

- Al_{13}^-

Al	0.000000000	0.000000000	2.667291000
Al	2.268933000	0.737221000	1.192849000
Al	2.268933000	-0.737221000	-1.192849000
Al	1.402278000	-1.930070000	1.192849000
Al	-1.402278000	-1.930070000	1.192849000
Al	-2.268933000	-0.737221000	-1.192849000
Al	-2.268933000	0.737221000	1.192849000
Al	0.000000000	2.385698000	1.192849000
Al	1.402278000	1.930070000	-1.192849000
Al	0.000000000	0.000000000	-2.667291000
Al	-1.402278000	1.930070000	-1.192849000
Al	0.000000000	-2.385698000	-1.192849000
Al	0.000000000	0.000000000	0.000000000

- Al_7H : **1o**

Al	-0.534660000	1.706700000	-0.000607000
Al	1.481194000	0.779739000	1.349313000
Al	1.481046000	-1.558978000	0.000555000
Al	-0.533929000	-0.853229000	-1.476554000
Al	1.481193000	0.778778000	-1.349868000
Al	-0.533929000	-0.852176000	1.477161000
Al	-2.523364000	-0.000656000	0.000001000
H	-4.128157000	-0.002315000	0.000003000

- Al_7H : **1b**

Al	0.244746000	0.858828000	1.614111000
Al	0.244746000	-1.729494000	1.265465000
Al	0.244746000	-1.729494000	-1.265465000
Al	0.244746000	0.858828000	-1.614111000
Al	2.097157000	0.115193000	0.000000000
Al	-1.670857000	-0.432290000	0.000000000
Al	-1.471145000	2.282138000	0.000000000
H	0.856213000	-2.908206000	0.000000000

- $Al_{13}H$: **1f**

Al	1.324625000	-2.283652000	-0.576942000
Al	1.661010000	0.005402000	-2.079928000
Al	-0.854295000	1.445808000	-2.065586000
Al	-0.844872000	-1.451335000	-2.065586000
Al	-1.300801000	-2.276597000	0.535669000
Al	-1.675278000	-0.005448000	2.047908000
Al	0.861602000	-1.458842000	2.034516000
Al	2.626530000	0.008542000	0.512462000
Al	1.309743000	2.292221000	-0.576942000
Al	-1.315582000	2.268087000	0.535669000
Al	0.852094000	1.464415000	2.034516000
Al	-2.645413000	-0.008604000	-0.552579000
Al	-0.000314000	-0.000001000	-0.015367000
H	0.012358000	0.000040000	3.018440000

- $Al_{13}H$: **1o**

Al	-2.345684000	-0.704522000	1.119236000
Al	-0.000003000	-0.000133000	2.559607000
Al	2.311213000	-0.810481000	1.119236000
Al	-0.055709000	-2.448417000	1.119331000
Al	-1.461031000	-1.917973000	-1.208204000
Al	0.000006000	0.000260000	-2.493732000
Al	-2.275736000	0.797593000	-1.207556000
Al	-1.395394000	2.012807000	1.120654000
Al	1.485498000	1.947258000	1.120654000
Al	2.309658000	0.693262000	-1.207556000
Al	0.054883000	2.412111000	-1.207085000
Al	1.372285000	-1.982440000	-1.208204000
Al	0.000022000	0.000984000	0.054563000
H	-0.000091000	-0.004001000	4.147731000

- $Al_{13}H_3$: **2o1b**

Al	-2.579491000	0.000015000	0.726149000
Al	-0.338066000	1.440662000	2.175381000
Al	-0.337944000	-1.440879000	2.175321000
Al	-1.392155000	2.291304000	-0.204198000
Al	-1.392093000	-2.291309000	-0.204237000
Al	-1.918869000	-0.000091000	-1.893055000
Al	-0.017931000	-0.000003000	0.000075000
Al	2.047219000	0.000063000	1.729688000
Al	1.421789000	2.292726000	0.276081000
Al	1.421999000	-2.292567000	0.276031000
Al	0.354494000	1.506686000	-2.141781000
Al	0.354638000	-1.506753000	-2.141731000

Al	2.443021000	0.000157000	-1.014581000
H	-3.902734000	-0.000143000	1.619261000
H	3.919059000	0.000119000	-1.617510000
H	-0.882280000	-0.000133000	3.129375000

- $Al_{13}H_3$: **1o2b**

Al	2.674535000	-0.895779000	0.535019000
Al	-0.197105000	-1.286114000	2.274671000
Al	1.341516000	1.063358000	1.995964000
Al	0.590887000	-2.624022000	0.078686000
Al	2.153956000	1.634559000	-0.572851000
Al	1.591100000	-0.761462000	-2.052942000
Al	0.034610000	-0.018437000	0.004472000
Al	-1.857344000	0.884256000	1.730857000
Al	-2.157541000	-1.584326000	0.467856000
Al	-0.287369000	2.655725000	0.506042000
Al	-0.966218000	-1.568942000	-1.932691000
Al	-0.018988000	1.513803000	-2.069216000
Al	-2.523380000	0.768005000	-0.926765000
H	-3.977525000	1.244403000	-1.419068000
H	0.735678000	-0.084225000	3.235556000
H	-1.680716000	1.691707000	-2.324807000

- Al_7I : **1o**

Al	1.288531000	1.731485000	-0.000855000
Al	3.288683000	0.781888000	1.353903000
Al	3.287575000	-1.564828000	0.000774000
Al	1.287630000	-0.865370000	-1.497492000
Al	3.288683000	0.780551000	-1.354673000
Al	1.287628000	-0.863888000	1.498344000
Al	-0.682202000	0.000877000	-0.000002000
I	-3.200092000	-0.000175000	0.000000000

- Al_7I : **1b**

Al	0.256237000	2.361384000	-1.661036000
Al	0.256237000	-0.235860000	-1.314246000
Al	0.256237000	-0.235860000	1.314246000
Al	0.256237000	2.361384000	1.661036000
Al	-1.541605000	1.549873000	0.000000000
Al	2.200424000	0.896332000	0.000000000
Al	1.920953000	3.552610000	0.000000000
I	-0.884177000	-2.514117000	0.000000000

- $Al_{13}I$: **1b**

Al	-0.269482000	-0.051134000	2.341457000
Al	-1.105586000	-1.451001000	-0.215550000
Al	-0.060909000	0.057593000	-2.432333000
Al	-1.100034000	1.469409000	-0.167045000
Al	0.880133000	2.251391000	1.496060000
Al	3.218126000	1.620398000	0.204044000
Al	2.502798000	-0.053387000	2.282952000
Al	0.884607000	-2.314189000	1.395829000
Al	1.124278000	-2.246410000	-1.540284000
Al	2.714212000	0.039685000	-2.102555000
Al	3.213501000	-1.634867000	0.121044000
Al	1.149263000	2.311720000	-1.441799000
Al	1.080401000	0.000882000	0.010606000
I	-3.490698000	-0.000022000	0.011669000

- $Al_{13}I$: **1o**

Al	0.000000000	2.453930000	-0.073994000
Al	0.000000000	0.000000000	1.370421000
Al	-1.442384000	-1.985271000	-0.073994000
Al	-2.333826000	0.758306000	-0.073994000
Al	-1.419645000	1.953974000	-2.400238000
Al	0.000000000	0.000000000	-3.685265000
Al	1.419645000	1.953974000	-2.400238000
Al	2.333826000	0.758306000	-0.073994000
Al	1.442384000	-1.985271000	-0.073994000
Al	0.000000000	-2.415245000	-2.400238000
Al	2.297035000	-0.746352000	-2.400238000
Al	-2.297035000	-0.746352000	-2.400238000
Al	0.000000000	0.000000000	-1.137673000
I	0.000000000	0.000000000	3.881279000

Figure S1. Molecular orbital (MO) diagrams for Al_7^- and **1o** Al_7H (H: HOMO and L: LUMO).

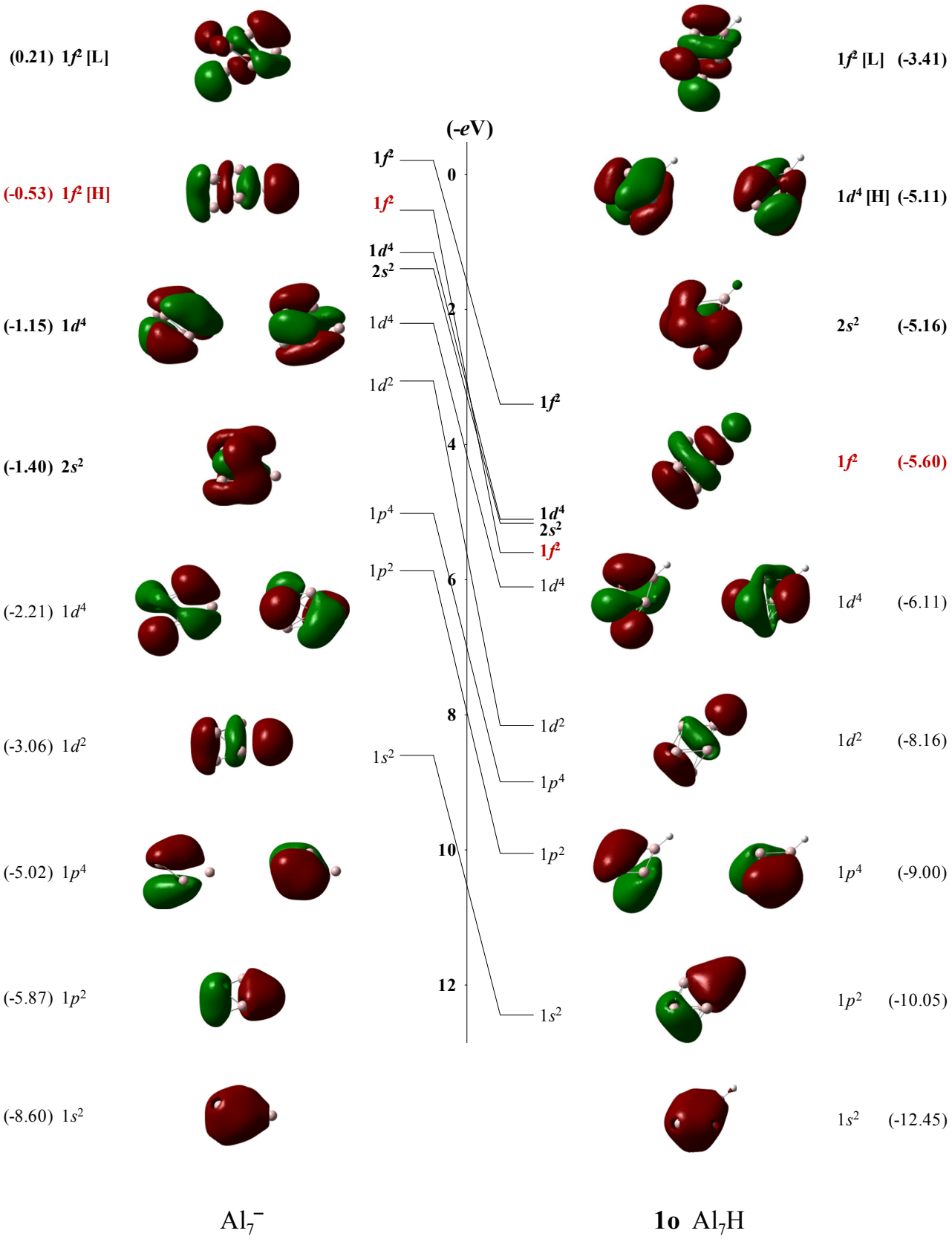


Figure S2. Molecular orbital (MO) diagrams for Al_7^- and **1b** Al_7H (H: HOMO and L: LUMO).

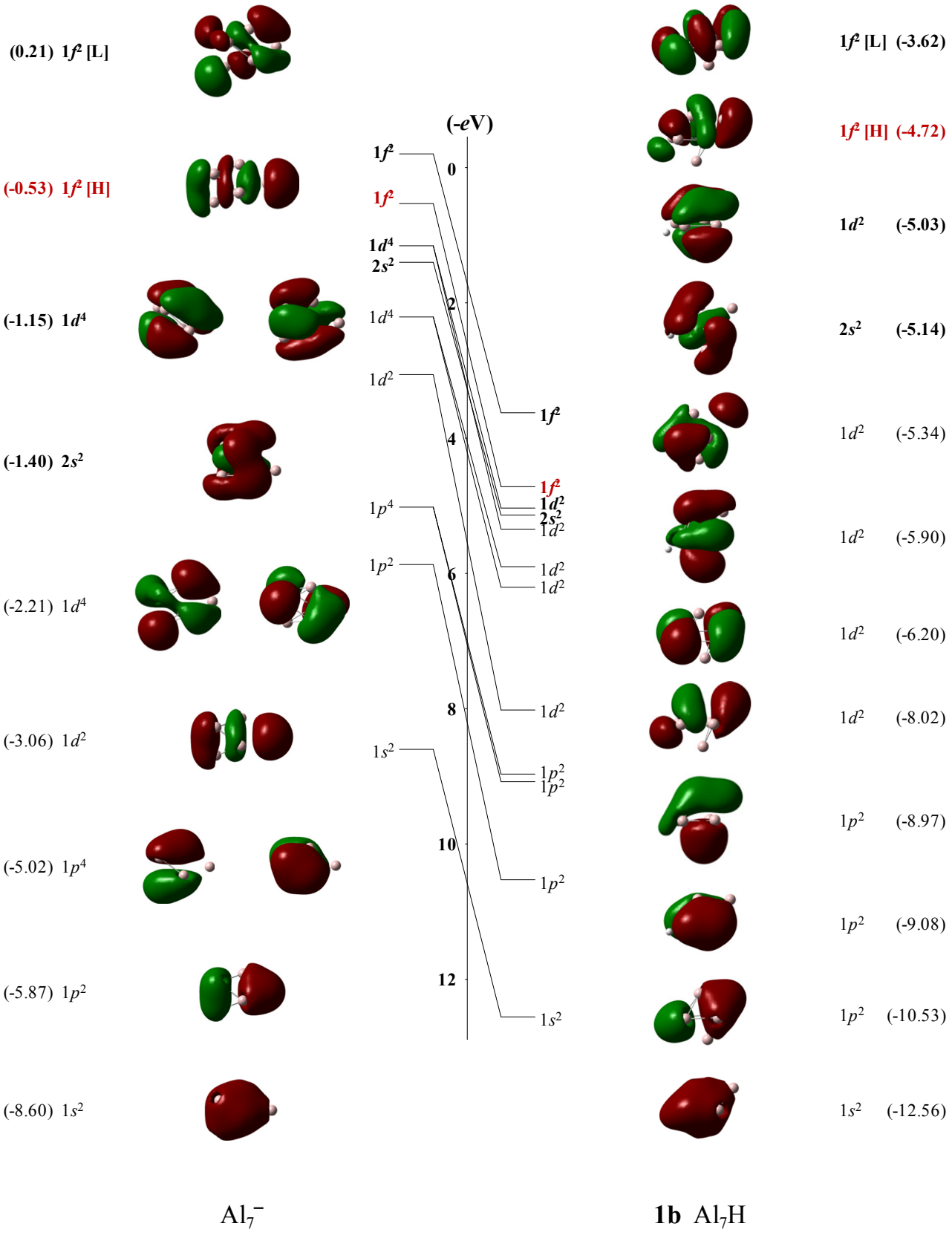


Figure S3. Molecular orbital (MO) diagrams for Al_{13}^- and **1f** $Al_{13}H$ (H: HOMO and L: LUMO).

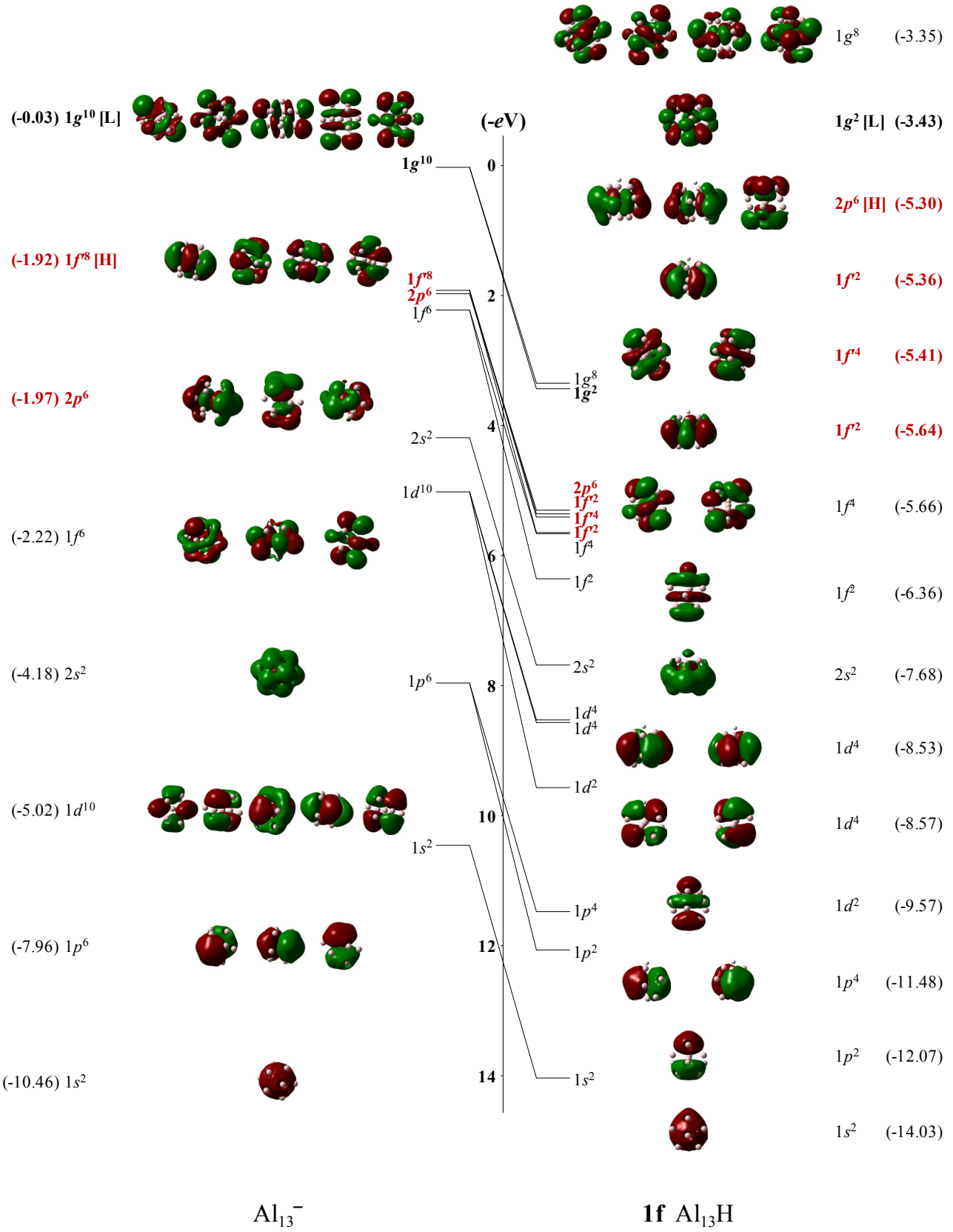


Figure S4. Molecular orbital (MO) diagrams for Al_{13}^- and **1o** $Al_{13}H$ (H: HOMO and L: LUMO).

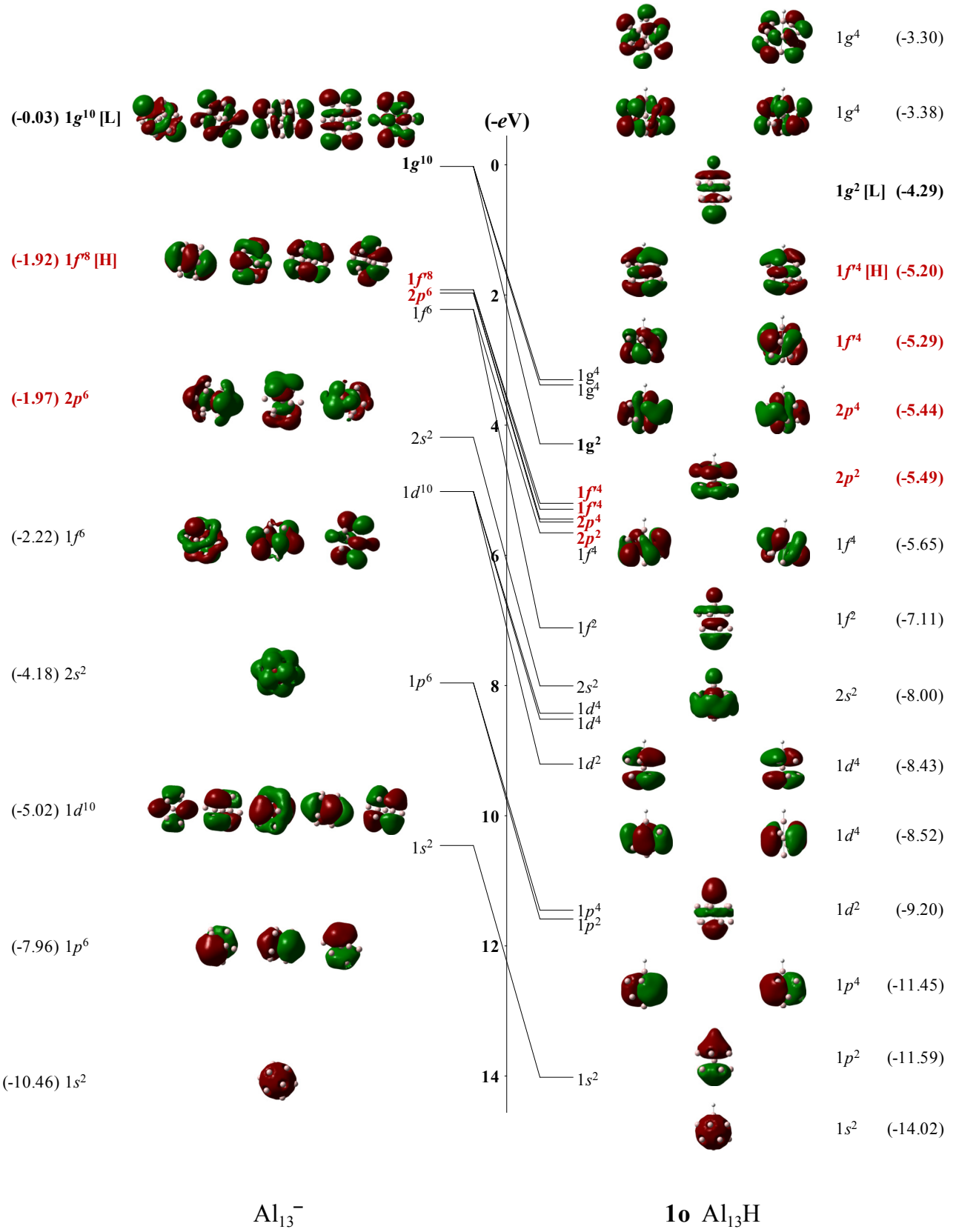
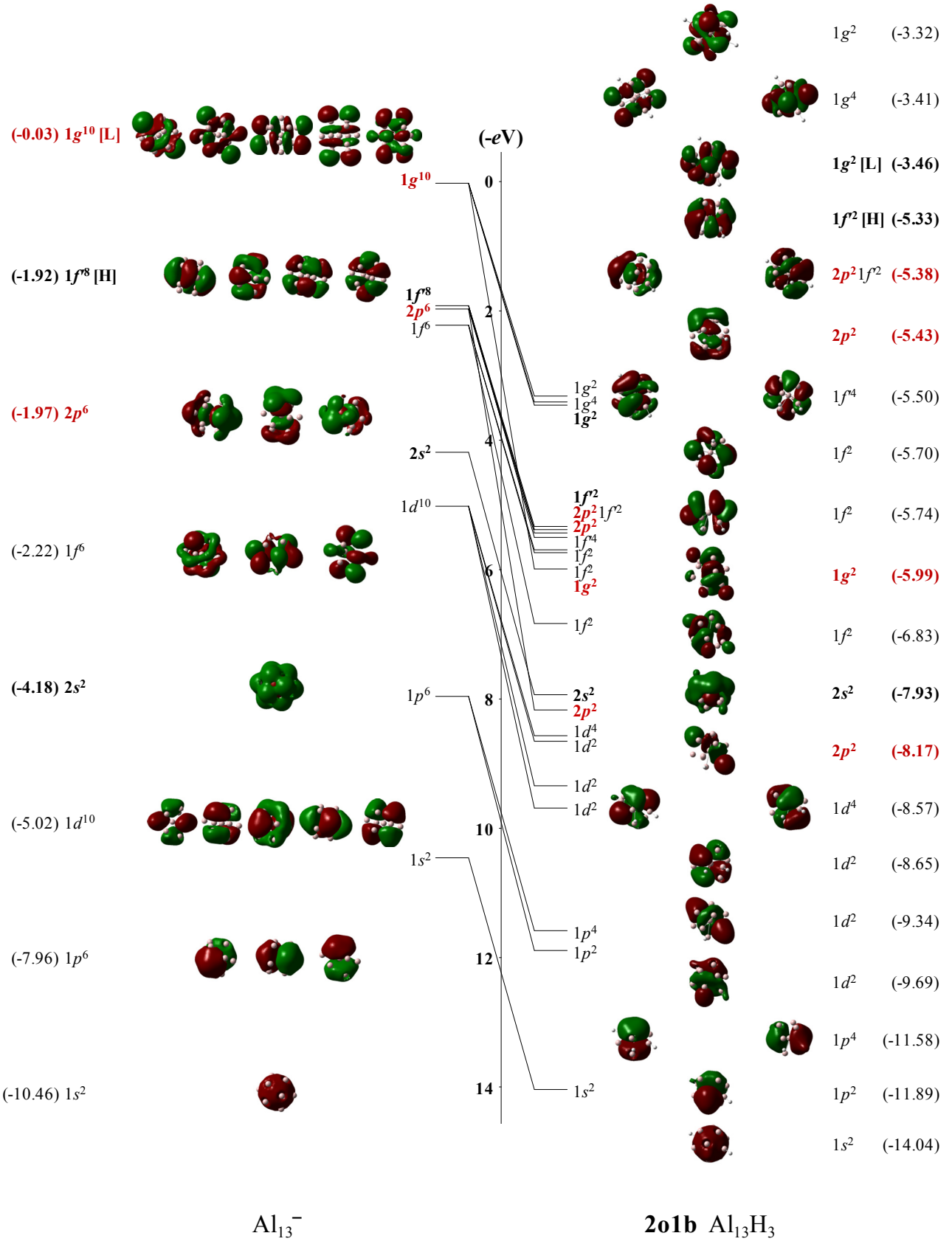
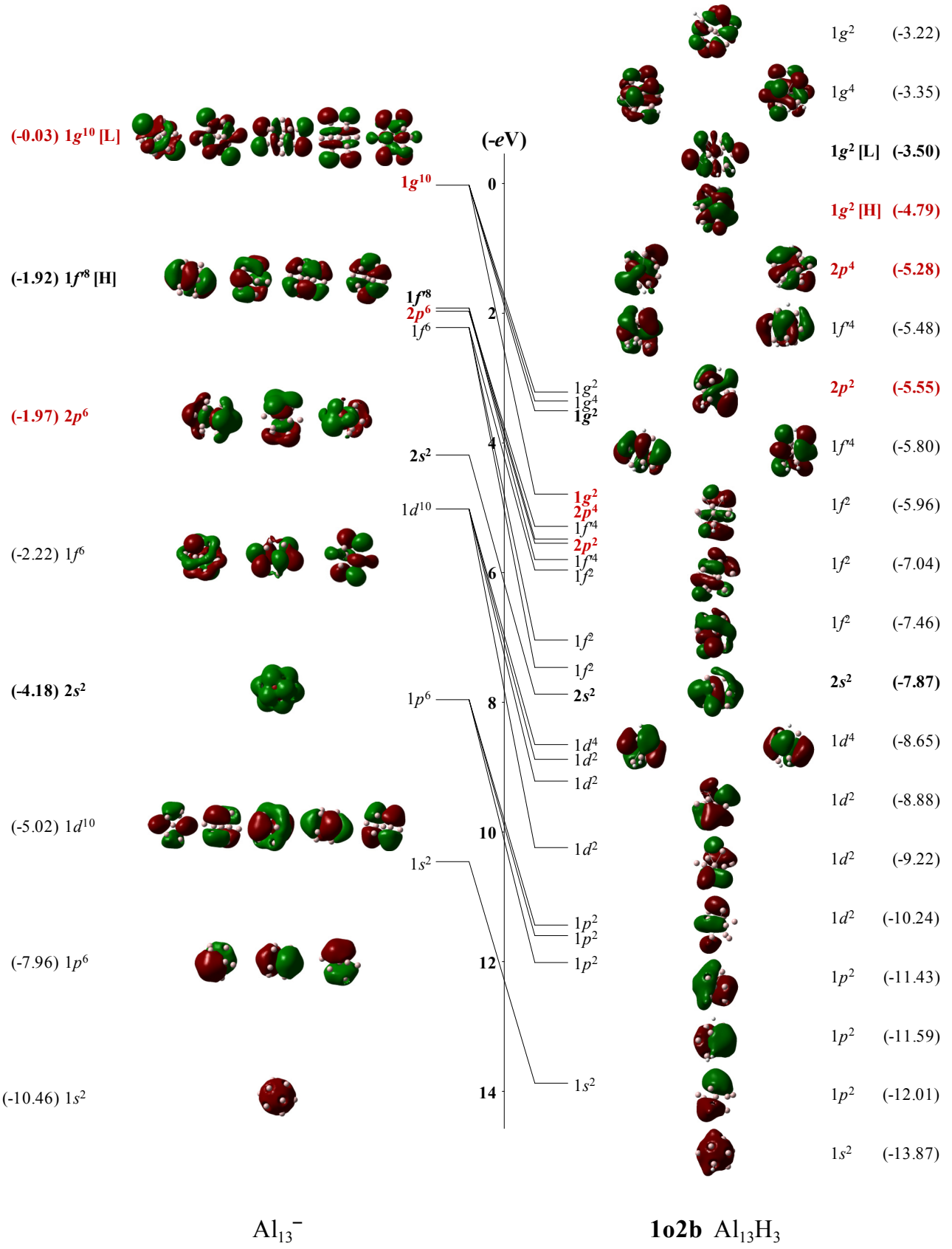


Figure S5. Molecular orbital (MO) diagrams for Al_{13}^- and **2o1b** $Al_{13}H_3$ (H: HOMO and L: LUMO).



Al_{13}^- **2o1b** $Al_{13}H_3$

Figure S6. Molecular orbital (MO) diagrams for Al_{13}^- and **1o2b** $Al_{13}H_3$ (H: HOMO and L: LUMO).



Al_{13}^- **1o2b** $Al_{13}H_3$