Al_2B_7. An Extension to the Inverse Sandwich B_9 Cluster Featuring Lewis Acid Sites And Planar Aromaticity

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Content

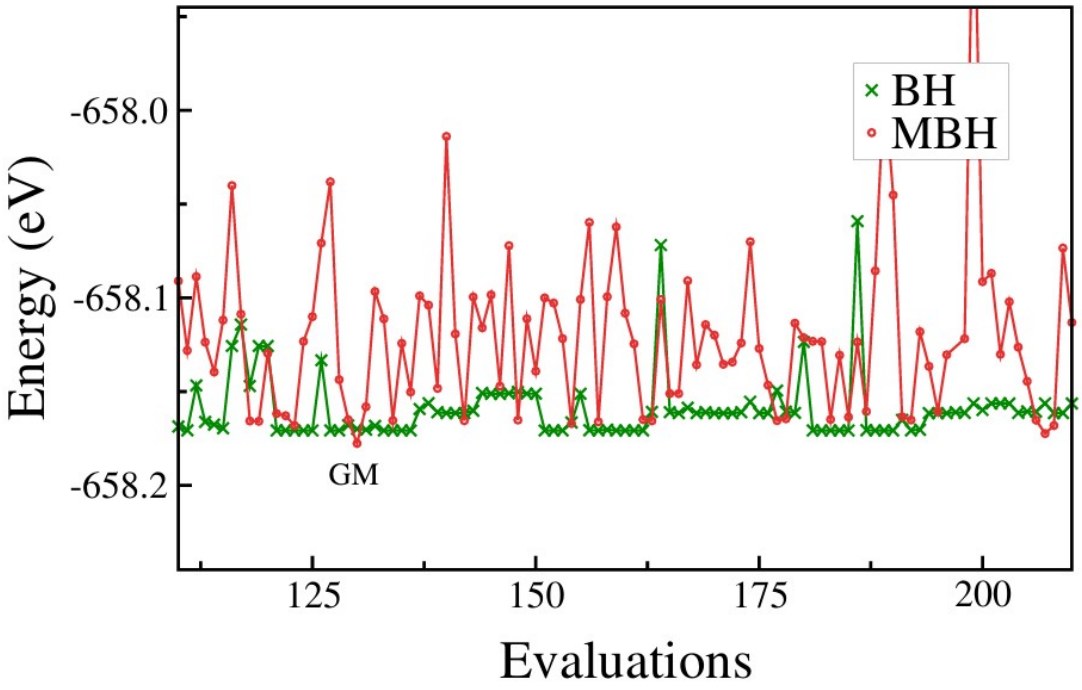

Figure S1. Potential energy surface for standard basing hopping (BH) and modified basing hopping (MBH) for Al_2B_7 clusters.

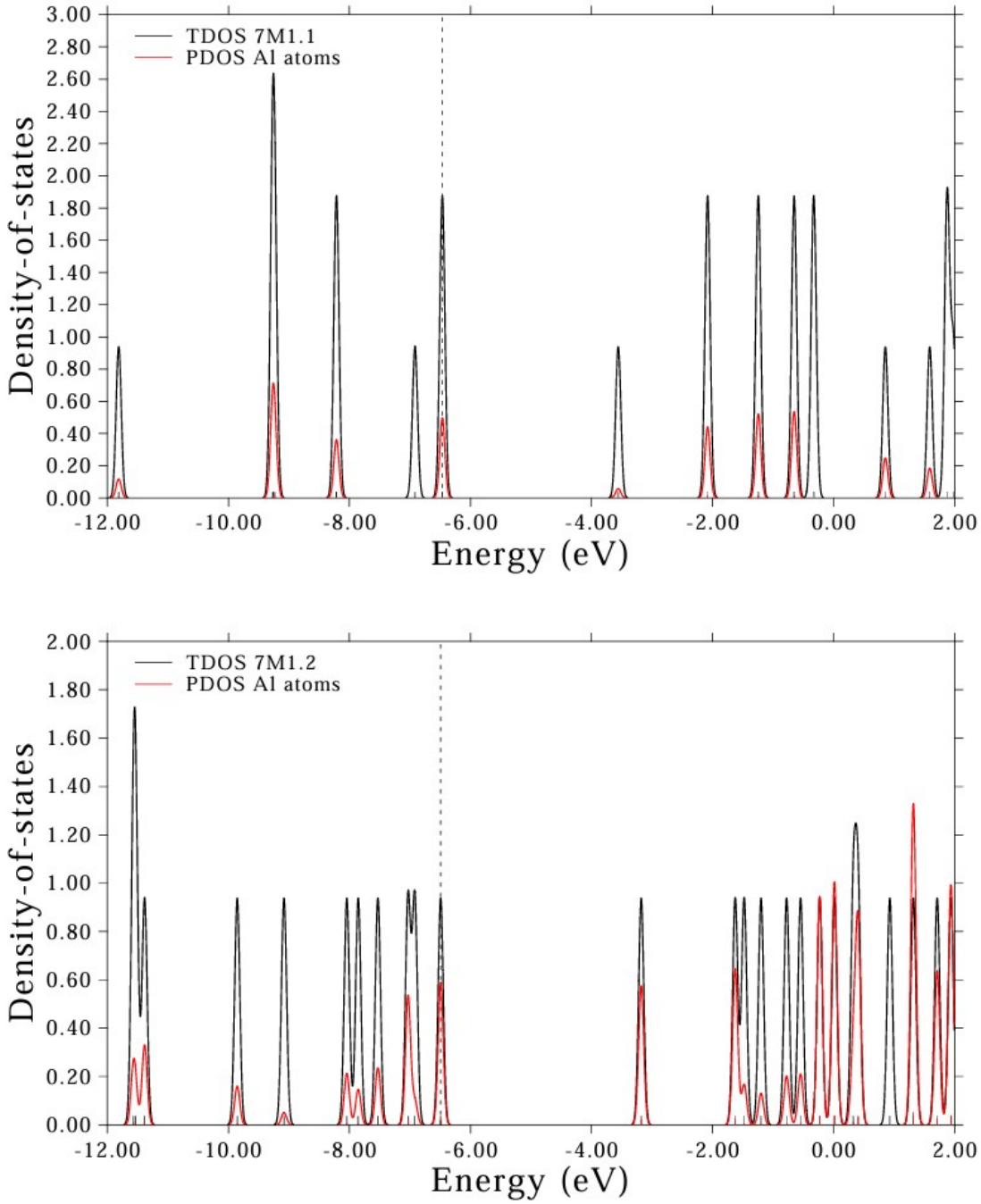

Figure S2. The total and partial density of states (TDOS, PDOS) for 7M2.1 and 7M2.2 clusters.The vertical dashed line corresponds to the Highest Occupied Molecular Orbital (HOMO) energy level.

Table S1. Energy decomposition analysis for the $^2B_2^+/^1B_7^-$, $^2Al_2^+/^1B_7^-$and $^2Al_2^{3+}/^1B_7^{3-}$ fragment interaction, in the respective B_9 and Al_2B_7 clusters. Values in kcal/mol, providing the percentage contribution from stabilizing terms. The Pauli term, accounts for the repulsion between occupied orbitals from fragments. The elstat and orb terms, are related to both electrostatic and orbital interaction nature of the interaction, with the disp term, accounting for London dispersion interactions, via the Grimme DFT-D3(BJ) correction to DFT.

	$^2B_2^+/^1B_7^-$		$^2Al_2^+/^1B_7^-$		$^2Al_2^+/^1B_7^{3-}$	
ΔE_{Pauli}	751.1		794.3		902.4	
ΔE_{elstat}	-652.4	38.2%	-840.8	50.4%	-1356.7	62.2%
ΔE_{orb}	-1056.4	61.8%	-828.5	49.6%	-825.2	37.8%
$\Delta E_{disp.}$		0.0%	-0.6	0.0%	-0.6	0.0%
ΔE_{int}	-957.8		-875.6		-1280.2	

Table S2. Wiberg bond orders for the capping B_2 and Al_2 motifs within the studied nine-vertex clusters, B_9 and Al_2B_7, respectively. In addition, other bond order schemes were included for comparison.

	B-B	Al-Al
Wiberg	0.37	0.13
Mayer	0.54	0.41
G-J[a]	0.51	0.35
N-M[b]	0.51	0.26

[a]Gopinathan-Jug bond order. [b]Nalewajski-Mrozek-3 bond order.

Table S3. Optimized coordinates for the studied clusters in a MultiXYZ format. Values in Angstroms (Å).

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9
B9
B         0.056501000      0.008135000      0.841265000
B        -0.032948000     -0.005399000     -0.860036000
B         1.112172000      1.382575000     -0.079949000
B         1.776364000      0.000999000     -0.102980000
B        -1.576556000      0.768191000      0.077605000
B        -0.380199000      1.723118000      0.000395000
B         1.113182000     -1.380640000     -0.058606000
B        -0.379135000     -1.719969000      0.028314000
B        -1.575988000     -0.764642000      0.089806000
9
B9 q=1+
B        -0.330512000      0.096063000      0.760269000
B         0.301827000     -0.076514000     -0.740056000
B         1.114575000      1.340725000     -0.056006000
B         1.917592000     -0.024926000     -0.130023000
B        -1.742208000      0.843376000      0.092377000
B        -0.408736000      1.703790000      0.037468000
B         1.169839000     -1.438894000     -0.116680000
B        -0.386800000     -1.634348000      0.002804000
B        -1.687123000     -0.754755000      0.094681000
9
Al2B7
Al        0.083572000      0.011292000      1.289088000
Al       -0.057773000     -0.008587000     -1.309108000
B         1.158853000      1.440787000     -0.079022000
B         1.853473000      0.001064000     -0.109221000
B        -1.645370000      0.800947000      0.077793000
B        -0.396876000      1.795743000      0.002990000
B         1.159127000     -1.437913000     -0.056626000
B        -0.396251000     -1.793120000      0.029641000
B        -1.645365000     -0.797847000      0.090280000
9
Al2B7 q=1+
Al        0.134318000      0.313073000      1.225381000
Al        0.031036000     -0.233778000     -1.261867000
B         1.181703000      1.394160000     -0.371056000
B         1.860693000     -0.031940000     -0.082892000
B        -1.635959000      0.847211000     -0.124438000
B        -0.364216000      1.779875000     -0.383870000
B         1.166493000     -1.427681000      0.253436000
B        -0.395169000     -1.742153000      0.384793000
B        -1.653267000     -0.737002000      0.218008000
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