Electronic Supplementary Information: Observation of d-p hybridized aromaticity in lanthanum-doped boron clusters

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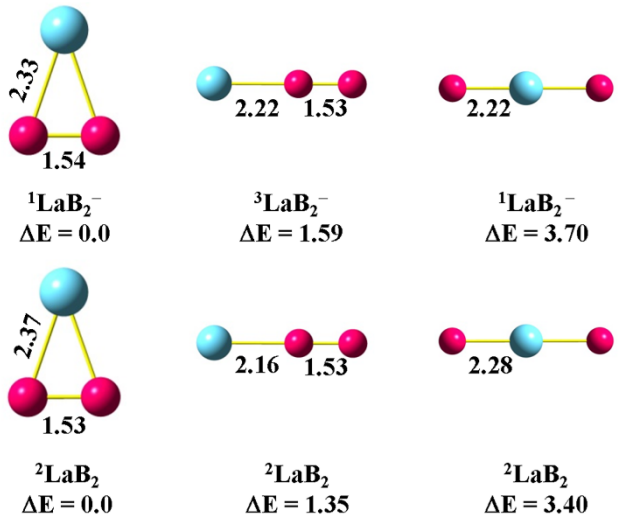
Figure S1. The calculated lowest-energy structures and low-lying states of anionic and neutral LaB_2 clusters determined at the B3LYP/SDDTZ level of theory. Bond lengths are given in angstroms (Å) and spin multiplicities are denoted as a superscript. The relative energies ΔE to the ground state are shown in eV.

Figure S2. The calculated lowest-energy structures and low-lying states of anionic and neutral LaB_3 clusters determined at the B3LYP/SDDTZ level of theory. Bond lengths are given in angstroms (Å) and spin multiplicities are denoted as a superscript. The relative energies ΔE to the ground state are shown in eV.

Figure S3. The calculated lowest-energy structures and low-lying states of anionic and neutral LaB_4 clusters determined at the B3LYP/SDDTZ level of theory. Bond lengths are given in angstroms (Å) and spin multiplicities are denoted as a superscript. The relative energies ΔE to the ground state are shown in eV.

Figure S4. Size dependence of the NICS values (in ppm) in neutral and anionic LaB_x (x = 2-4): (a) NICS values calculated at the ring center in the molecular plane, (b) NICS values calculated at 0.5 Å above the plane, and (c) NICS values calculated at 1.0 Å above the plane, respectively.

Figure S5. Occupied valence molecular orbitals of the LaB_3^-, LaB_4^-, LaB_2, and LaB_4 clusters. The isosurface value of the MOs is 0.04 au.



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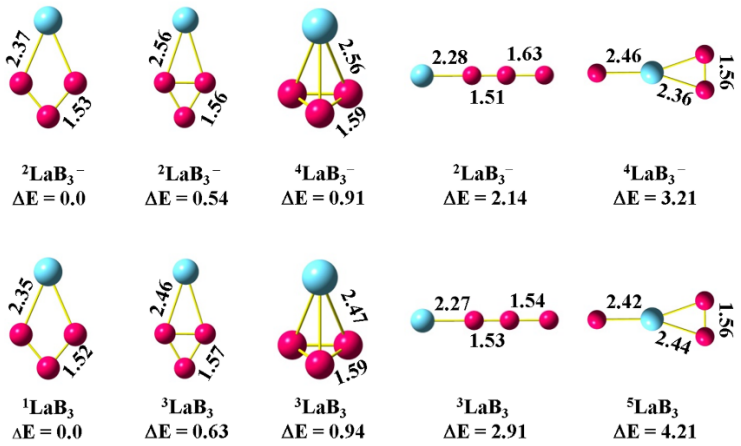

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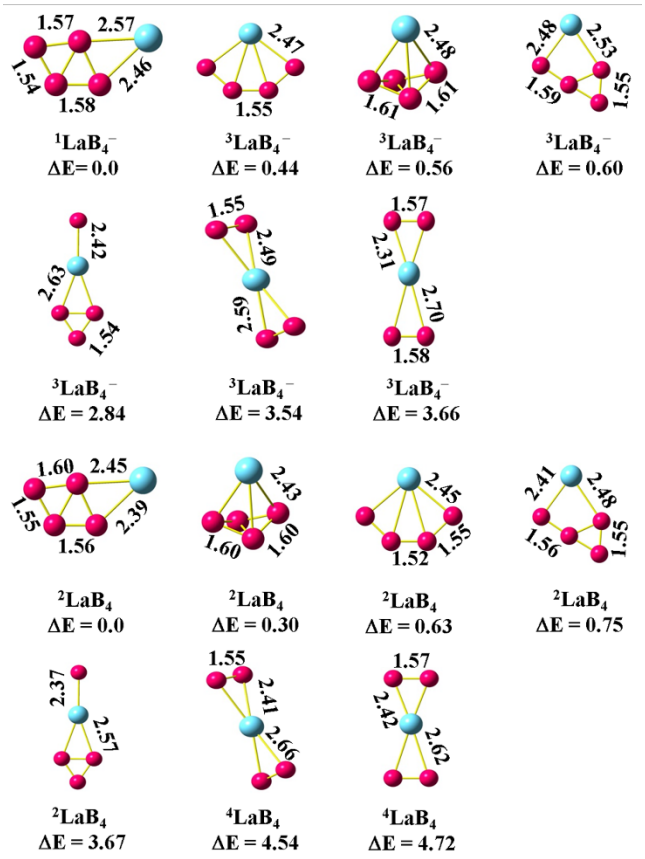

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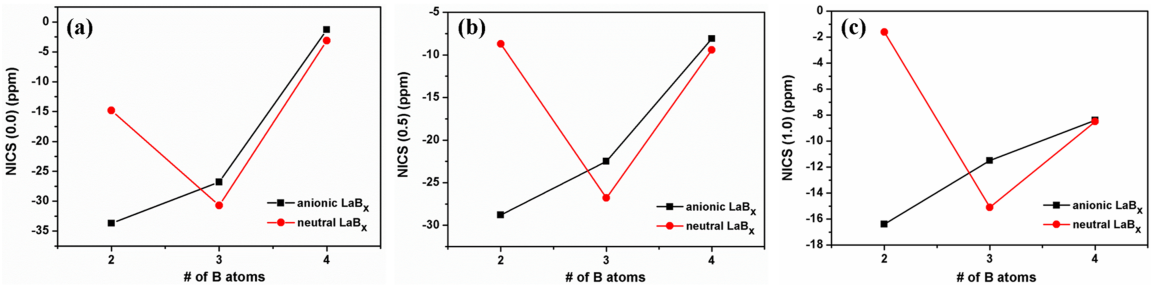

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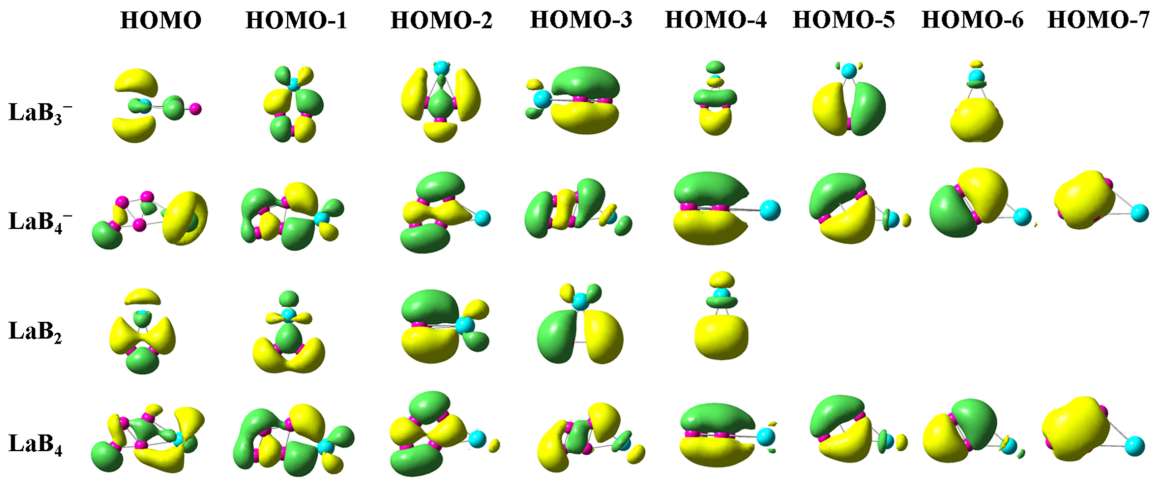

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