SUPPLEMENTARY INFORMATION

Why nanoscale tank treads move? Structures, chemical bonding, and molecular dynamics of a doped boron cluster $B_{10}C$†

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Supplementary Information – Part I

Table S1. Cartesian coordinates for the (C_s, $^1A'$) global-minimum (GM) and (C_{2v}, $^1A_1$) local-minimum (LM) structures of $B_{10}C$ at PBE0/6-311+G* level.

Figure S1. Alternative optimized structures of $B_{10}C$ cluster. Relative energies (in eV) are shown at the CCSD(T)/6-311G*//PBE0/6-311+G* and PBE0/6-311+G* (in square brackets) levels, and those at PBE0 level have been corrected for zero-point energies (ZPE).

Figure S2. Schematic structural evolution of the (C_{2v}, $^1A_1$) LM of $B_{10}C$, assuming in-plane rotation clockwise.

Figure S3. Canonical molecular orbitals (CMOs) of the (C_{2v}, $^1A_1$) LM structure of $B_{10}C$. (a) Nine localized σ bonds; (b) Five delocalized σ bonds; (c) Three delocalized π bonds. The 10σ and 6π electron-countings in (b) and (c) confirm to the ($4n$ + 2) Hückel rule for aromaticity.

Supplementary Information – Part II

Two short movies extracted from the BOMD simulations for the GM and LM structures of $B_{10}C$. Each frame of the snapshot is reoriented horizontally. The simulations were performed at 600 K for over 50 ps; and the movies roughly cover a time span of 3.5 ps.

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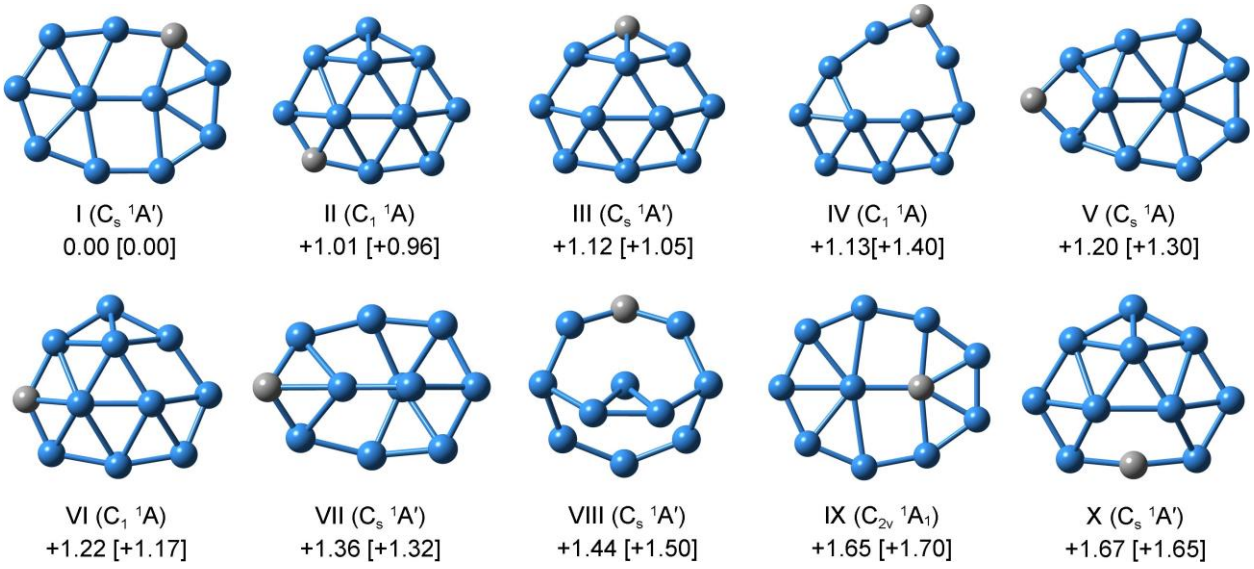

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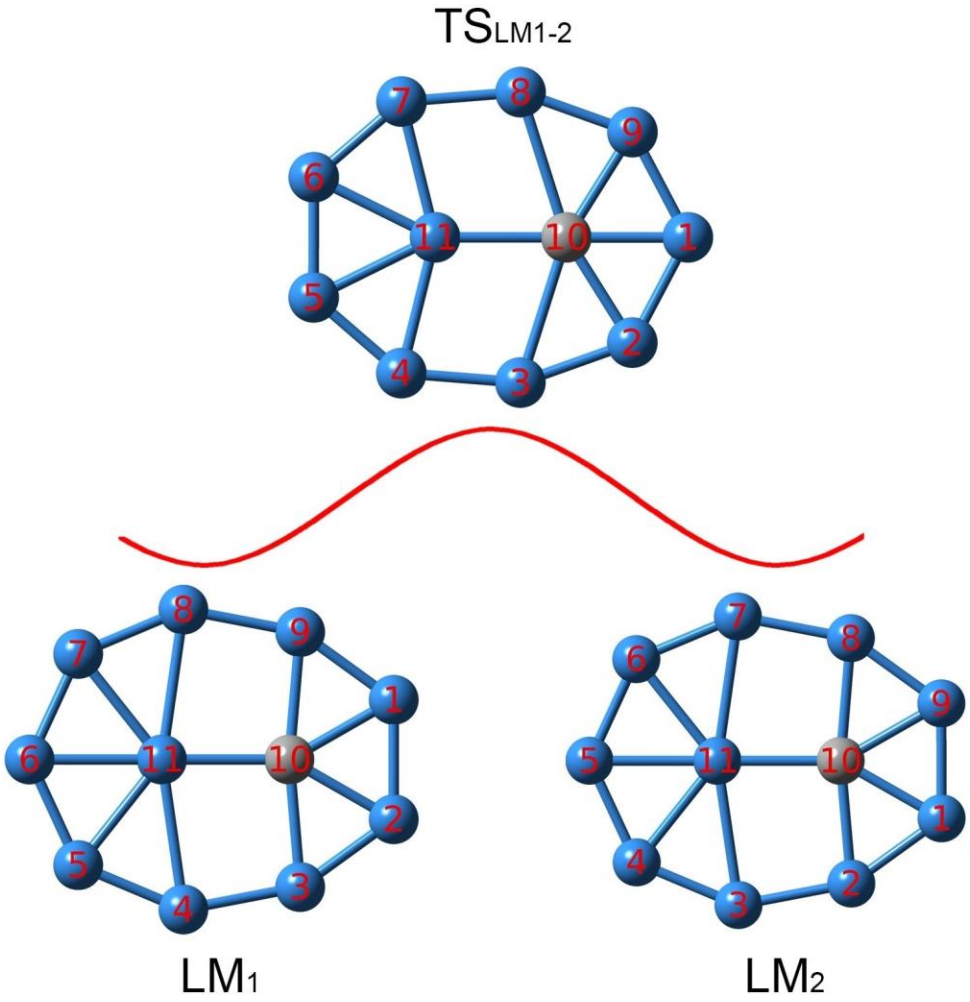

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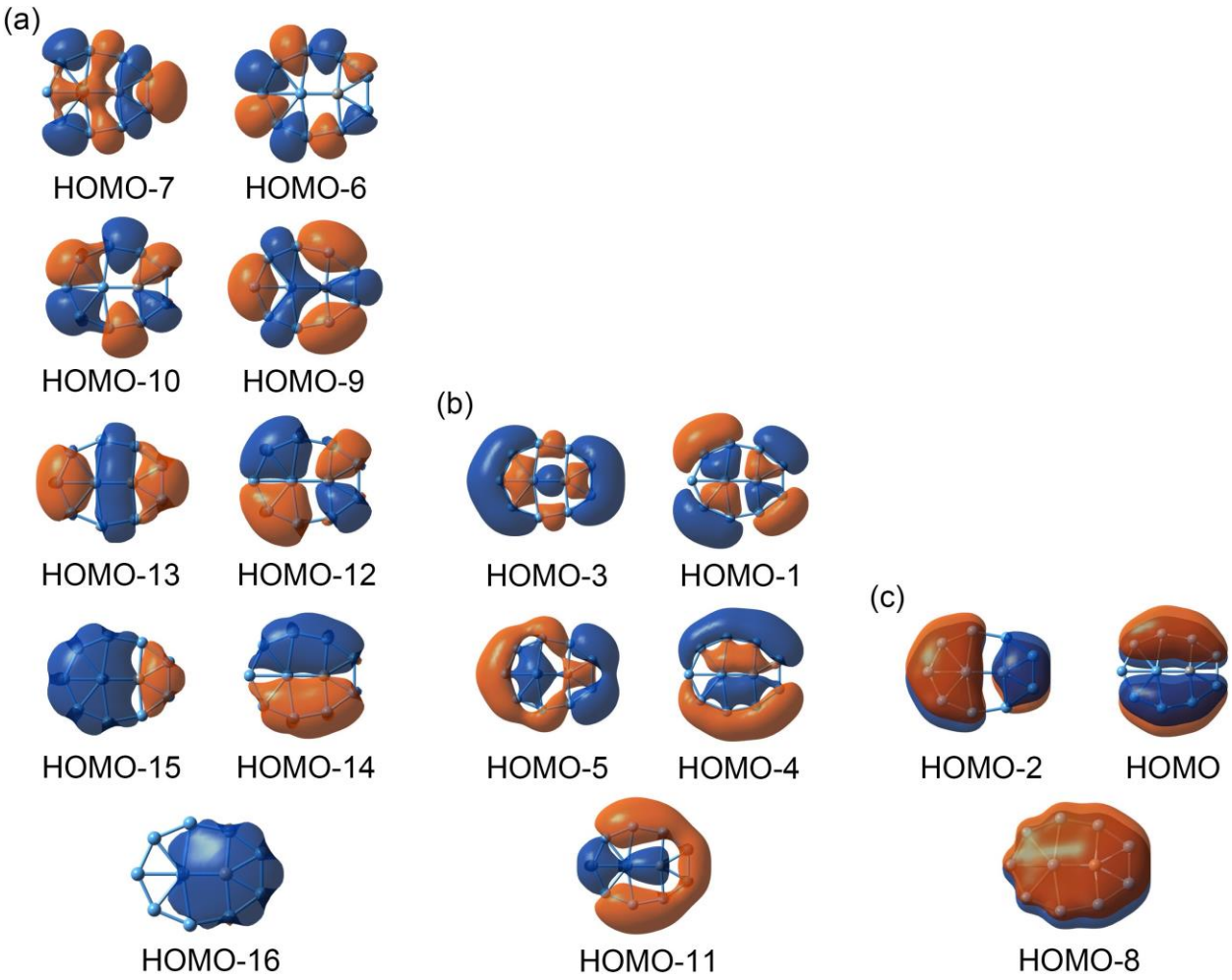

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(a) GM, C_s $B_{10}C$

B	-0.81933100	-0.03301105	0.00000000
B	-2.37663601	0.58133493	0.00000000
B	2.55748000	0.26213800	0.00000000
B	0.62531803	-1.80323703	0.00000000
B	-0.96495097	-1.82151005	0.00000000
B	0.91796000	-0.00527602	0.00000000
B	1.67957198	1.54104299	0.00000000
B	-2.23922699	-0.99418507	0.00000000
B	2.07864102	-1.23522401	0.00000000
B	0.11917998	1.69083097	0.00000000
C	-1.31500502	1.51424695	0.00000000

(b) LM, C_{2v} $B_{10}C$

B	0.00000000	1.68214500	1.07912000
B	0.00000000	-1.97896900	-0.46854400
B	0.00000000	1.39447800	-1.86288300
B	0.00000000	0.00000000	-2.50653600
B	0.00000000	0.78841500	2.31950800
B	0.00000000	-0.78841500	2.31950800
B	0.00000000	-1.39447800	-1.86288300
B	0.00000000	-1.68214500	1.07912000
B	0.00000000	0.00000000	-0.75217700
B	0.00000000	1.97896900	-0.46854400
C	0.00000000	0.00000000	0.93692600