Electronic Supplementary Material (ESI) for Nanoscale.

Supporting information

Predicting Lanthanide Boride Inverse Sandwich Tubular Molecular Rotors with the Smallest Core-Shell Structure†

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Fig. S1 Relative energies of low-lying isomers of $La_2[B_{18}]$ at CCSD(T) (square brackets), PBE0, and TPSSh (parentheses). Relative energies are given in eV.

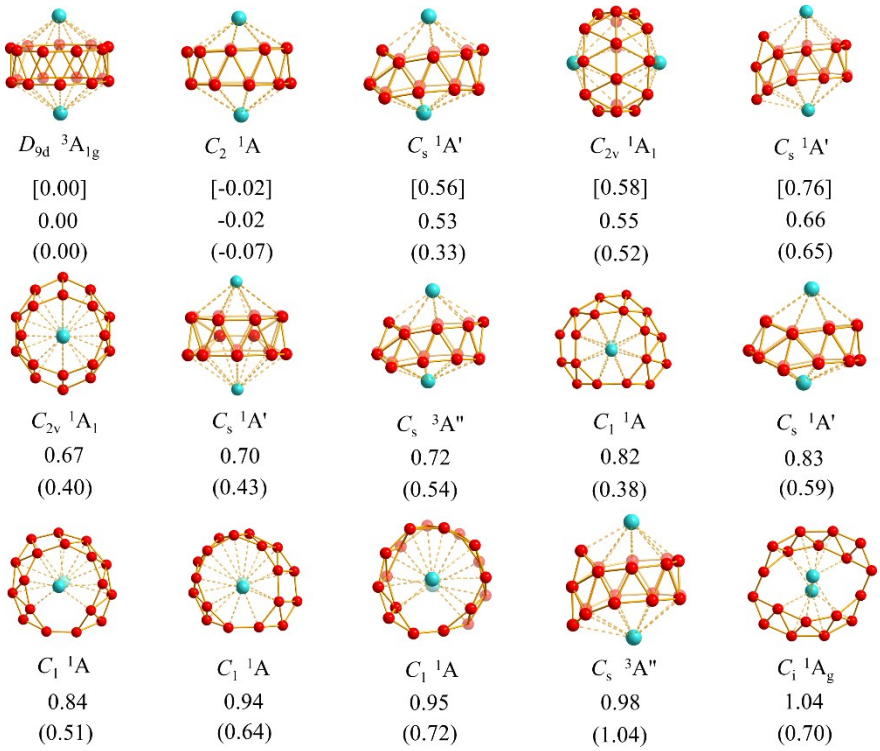

Fig. S2 Relative energies of low-lying isomers of $La_2[B_{18}]^-$ at PBE0 and TPSSh (parentheses). Relative energies are given in eV.

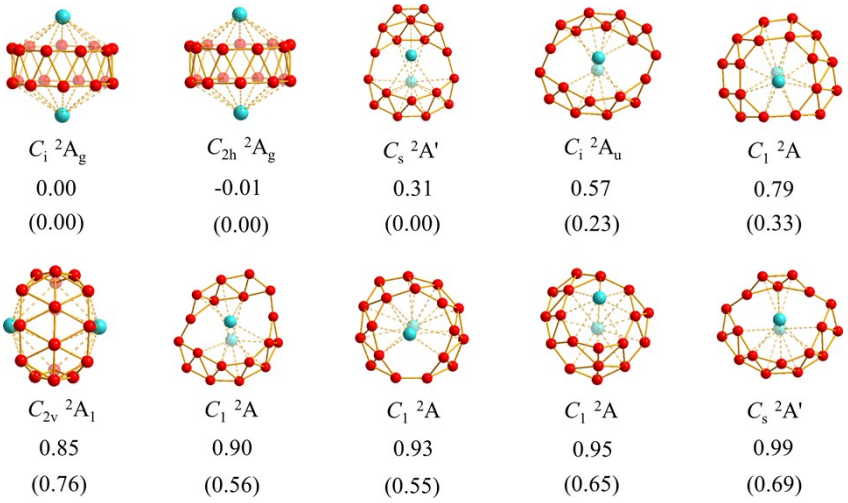

Fig. S3 Relative energies of low-lying isomers of $La_2[B_{18}]^{2-}$ at CCSD(T) (square brackets), PBE0, and TPSSh (parentheses). Relative energies are given in eV.

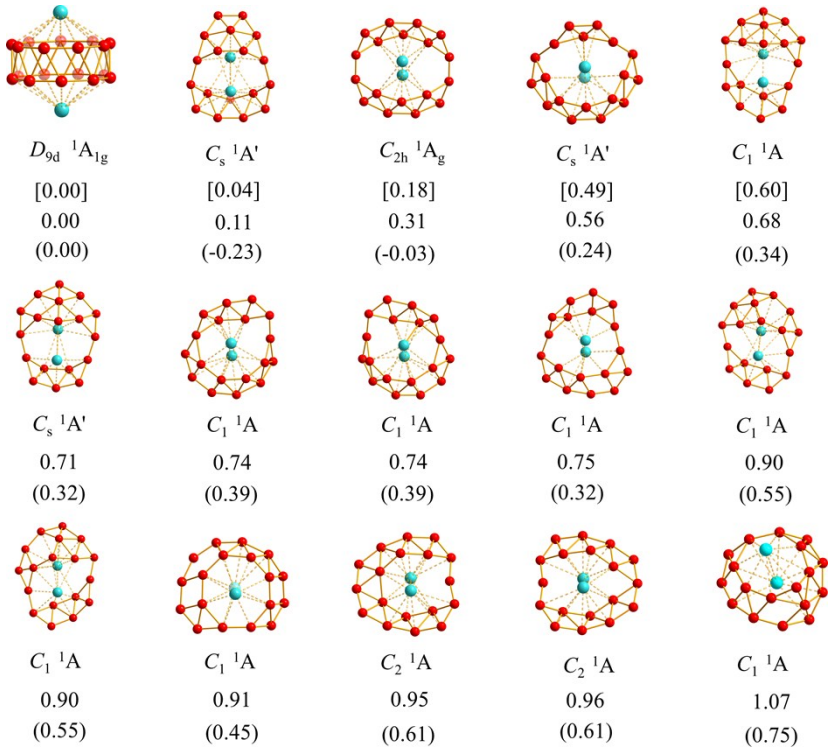

Fig. S4 Relative energies of low-lying isomers of $La_2[B_2@B_{18}]$ at CCSD(T) (square brackets), PBE0, and TPSSh (parentheses). Relative energies are given in eV.

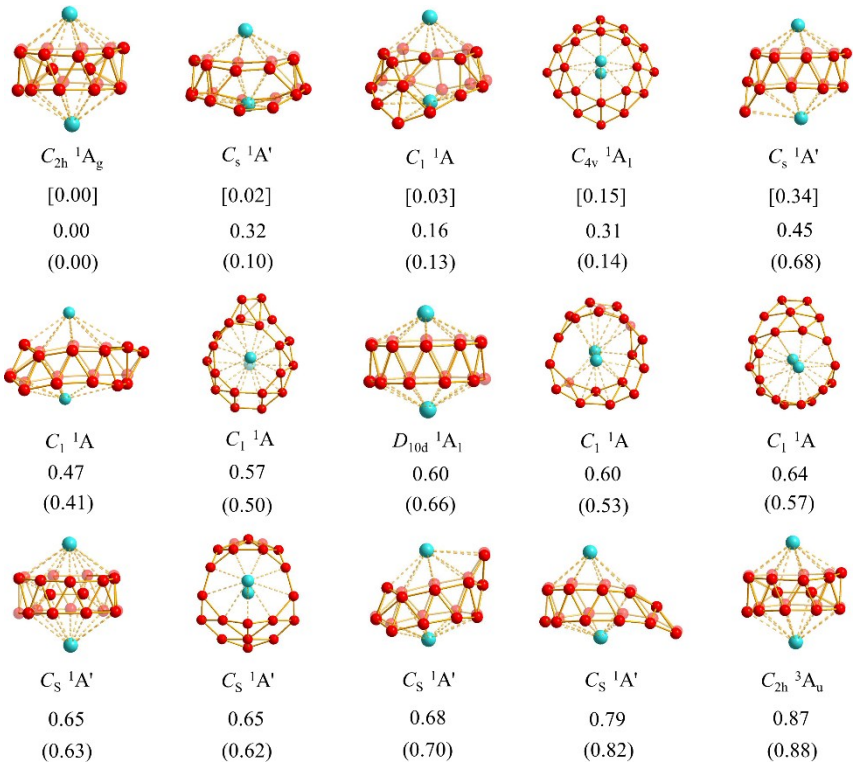

Fig. S5 Eigenvalue spectrum of C_{2h} $La_2[B_2@B_{18}]$ (**4**) with its CMOs related with the 6 12c-2e (d-p)σ bonds, 3 20c-2e σ bonds, 2 22c-2e (d-p)δ bonds, and 3 22c-2e (d-p)π bonds in Fig.3b depicted.

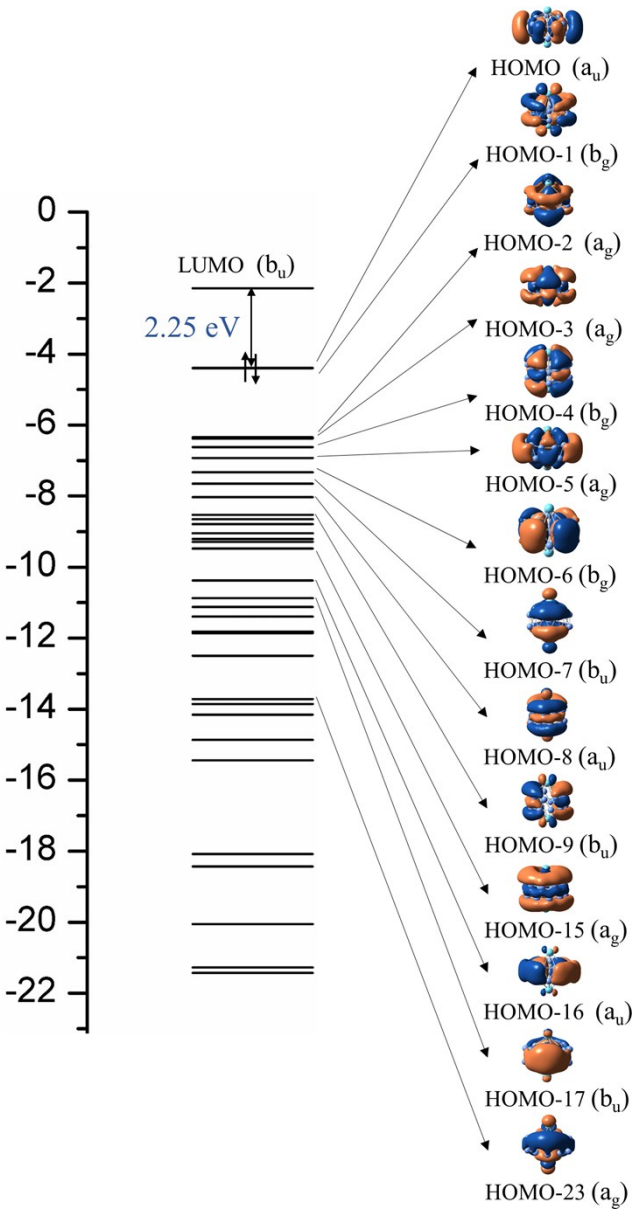

Fig. S6 Relative energies of low-lying isomers of $La_2[B_2@B_{18}]^+$ at PBE0 and TPSSh (parentheses). Relative energies are given in eV.

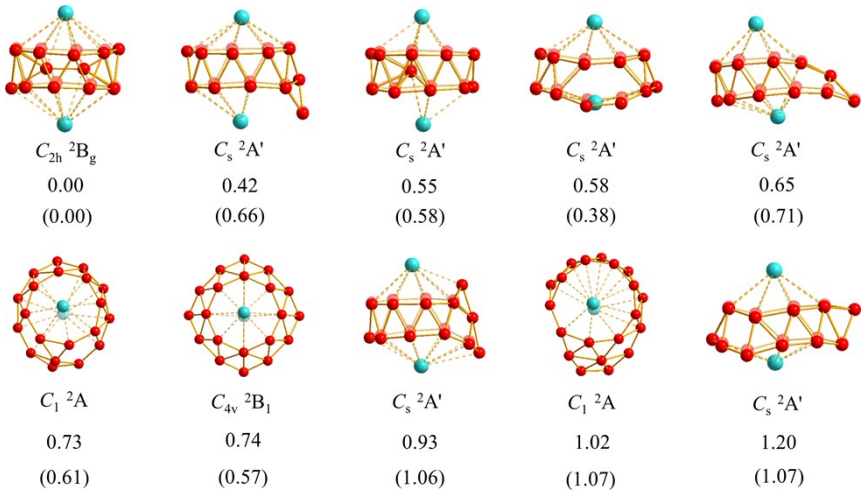

Fig. S7 The AdNDP bonding pattern of TS C_{2h} $La_2[B_2@B_{18}]$, with the occupation numbers (ONs) indicated.

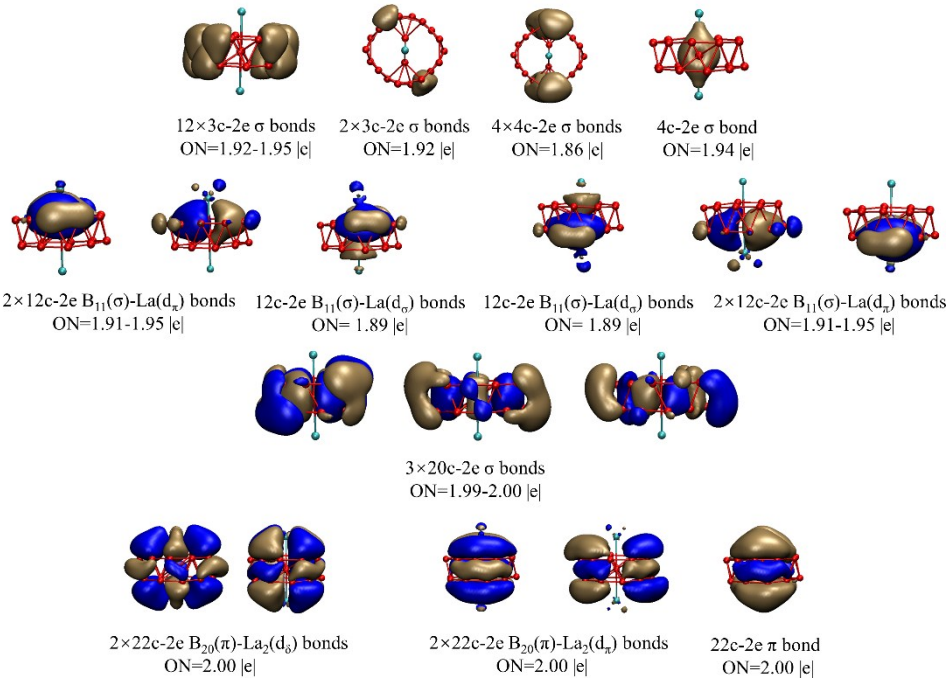

Table S1 Optimized coordinates (x, y, z) of D_{9d} $La_2[B_{18}]$ (**2**), D_{9d} $La_2[B_{18}]^{2-}$ (**3**), C_{2h} $La_2[B_2@B_{18}]$ (**4**) and TS C_{2h} $La_2[B_2@B_{18}]$ at PBE0/6-311+G(d) level.

D_{9d} $La_2[B_{18}]$ ($^3A_{1g}$) (**2**)

B	0.00000000	2.32533800	0.77566200
B	1.49469800	1.78131200	0.77566200
B	-2.29001100	0.40379100	0.77566200
B	-1.49469800	1.78131200	0.77566200
B	-0.79531200	-2.18510300	0.77566200
B	-2.01380200	-1.16266900	0.77566200
B	2.29001100	0.40379100	0.77566200
B	2.01380200	-1.16266900	0.77566200
B	0.79531200	-2.18510300	0.77566200
B	-2.29001100	-0.40379100	-0.77566200
B	-1.49469800	-1.78131200	-0.77566200
B	-0.79531200	2.18510300	-0.77566200
B	-2.01380200	1.16266900	-0.77566200
B	2.01380200	1.16266900	-0.77566200
B	0.79531200	2.18510300	-0.77566200
B	0.00000000	-2.32533800	-0.77566200
B	1.49469800	-1.78131200	-0.77566200
B	2.29001100	-0.40379100	-0.77566200
La	0.00000000	0.00000000	-2.29500100
La	0.00000000	0.00000000	2.29500100

D_{9d} $La_2[B_{18}]^{2-}$ ($^1A_{1g}$) (**3**)

B	0.00000000	2.32557000	0.79958100
B	1.49484700	1.78149000	0.79958100
B	-2.29023900	0.40383100	0.79958100
B	-1.49484700	1.78149000	0.79958100
B	-0.79539200	-2.18532100	0.79958100
B	-2.01400200	-1.16278500	0.79958100
B	2.29023900	0.40383100	0.79958100
B	2.01400200	-1.16278500	0.79958100
B	0.79539200	-2.18532100	0.79958100
B	-2.29023900	-0.40383100	-0.79958100
B	-1.49484700	-1.78149000	-0.79958100
B	-0.79539200	2.18532100	-0.79958100
B	-2.01400200	1.16278500	-0.79958100
B	2.01400200	1.16278500	-0.79958100
B	0.79539200	2.18532100	-0.79958100
B	0.00000000	-2.32557000	-0.79958100
B	1.49484700	-1.78149000	-0.79958100
B	2.29023900	-0.40383100	-0.79958100
La	0.00000000	0.00000000	-2.23507200
La	0.00000000	0.00000000	2.23507200

C_{2h} $La_2[B_2@B_{18}]$ (^1A_g) (**4**)

B	-0.77533200	1.07735100	1.99227500
B	-0.79669100	2.16270500	0.81637800
B	-0.79669100	2.16270500	-0.81637800
B	-0.77533200	1.07735100	-1.99227500
B	-0.72571700	-0.42221100	-2.57961500
B	-0.79669100	-1.68145200	-1.48716100
B	-0.90164200	-2.30723200	0.00000000
B	-0.79669100	-1.68145200	1.48716100
B	-0.72571700	-0.42221100	2.57961500
B	0.72571700	0.42221100	2.57961500
B	0.90164200	2.30723200	0.00000000
B	-0.00118700	0.81781300	0.00000000
B	0.79669100	1.68145200	-1.48716100
B	0.72571700	0.42221100	-2.57961500
B	0.77533200	-1.07735100	-1.99227500
B	0.79669100	-2.16270500	-0.81637800
B	0.00118700	-0.81781300	0.00000000
B	0.79669100	-2.16270500	0.81637800
B	0.77533200	-1.07735100	1.99227500
B	0.79669100	1.68145200	1.48716100
La	-2.39793100	0.03092300	0.00000000
La	2.39793100	-0.03092300	0.00000000

TS C_{2h} $La_2[B_2@B_{18}]$

B	-0.67716600	2.36052400	0.79091000
B	0.00000000	1.40010000	1.94349400
B	0.95184100	0.12189400	2.28349600
B	1.63194900	-1.01308200	1.38230700
B	2.07103900	-1.78197300	0.00000000
B	1.63194900	-1.01308200	-1.38230700
B	0.95184100	0.12189400	-2.28349600
B	0.00000000	1.40010000	-1.94349400
B	-0.67716600	2.36052400	-0.79091000
B	-2.07103900	1.78197300	0.00000000
B	-0.95184100	-0.12189400	2.28349600
B	0.00000000	0.00000000	0.81822500
B	0.00000000	-1.40010000	1.94349400
B	0.67716600	-2.36052400	0.79091000
B	0.67716600	-2.36052400	-0.79091000
B	0.00000000	-1.40010000	-1.94349400
B	0.00000000	0.00000000	-0.81822500
B	-0.95184100	-0.12189400	-2.28349600
B	-1.63194900	1.01308200	-1.38230700
B	-1.63194900	1.01308200	1.38230700
La	1.95910800	1.37179300	0.00000000
La	-1.95910800	-1.37179300	0.00000000