Supporting information

Perfect cubic La-doped boron clusters $La_6\&[La@B_{24}]^{+/0}$ as the embryos of low-dimensional lanthanide boride nanomaterials

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Fig. S1 Relative energies of low-lying isomers of $La_7B_{24}^+$ at PBE0 and TPSSh (parentheses) levels in eV.

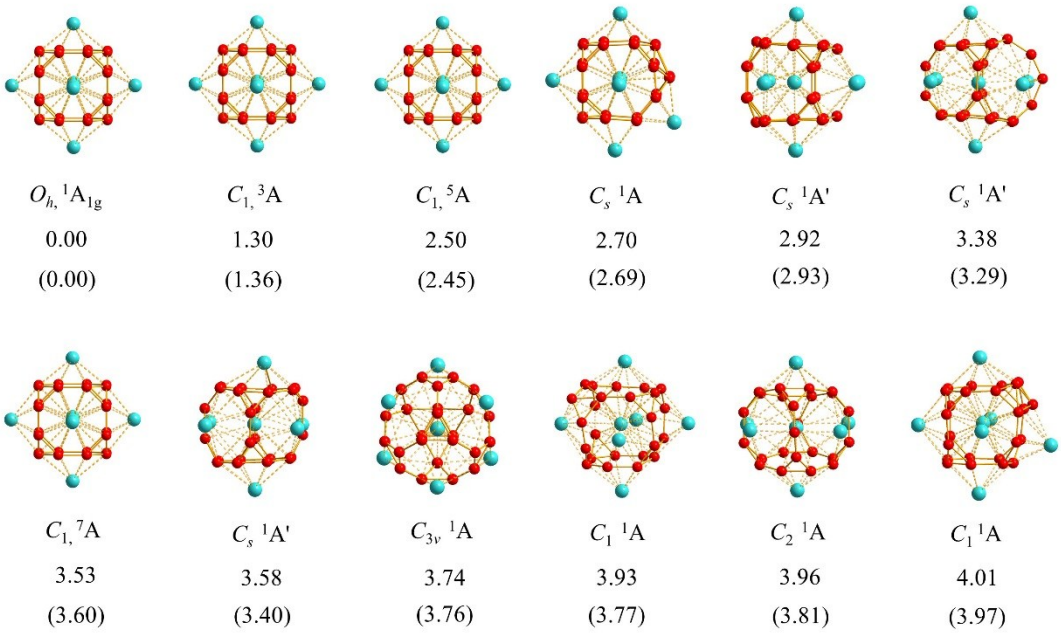
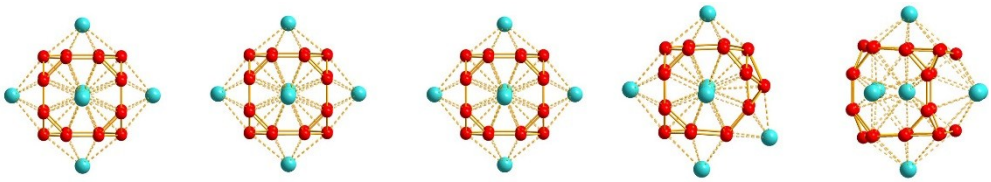
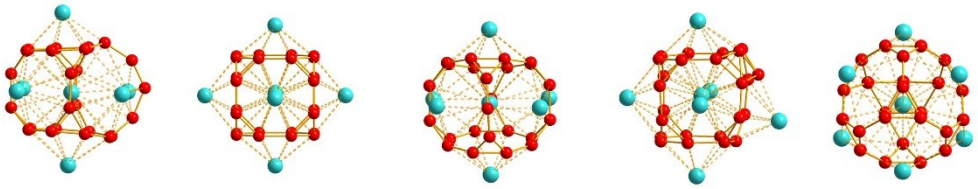


Fig. S2 Relative energies of low-lying isomers of La_7B_{24} at PBE0 and TPSSh (parentheses) levels in eV.



O_h, $^2A_{2g}$ | O_h, $^4A_{1g}$ | O_h, $^6A_{1g}$ | C_s $^2A''$ | C_s $^2A'$

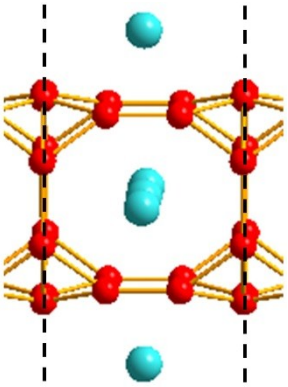
0.00 (0.00) | 1.22 (1.25) | 2.28 (2.42) | 2.41 (2.38) | 2.49 (2.50)



C_s $^2A'$ | O_h, $^8A_{1u}$ | C_2 ^2B | C_1 ^2A | C_1 ^2A

3.00 (2.87) | 3.26 (3.35) | 3.59 (3.43) | 3.90 (3.84) | 3.92 (3.90)

Fig. S3. The optimized structure of 1D La_5B_{16} nanowire



P4/mmm

Fig. S4 Relative energies per unit cell (eV) of the low-lying isomers of 1D $La_{10}B_{32}$ (**5**) nanowires.

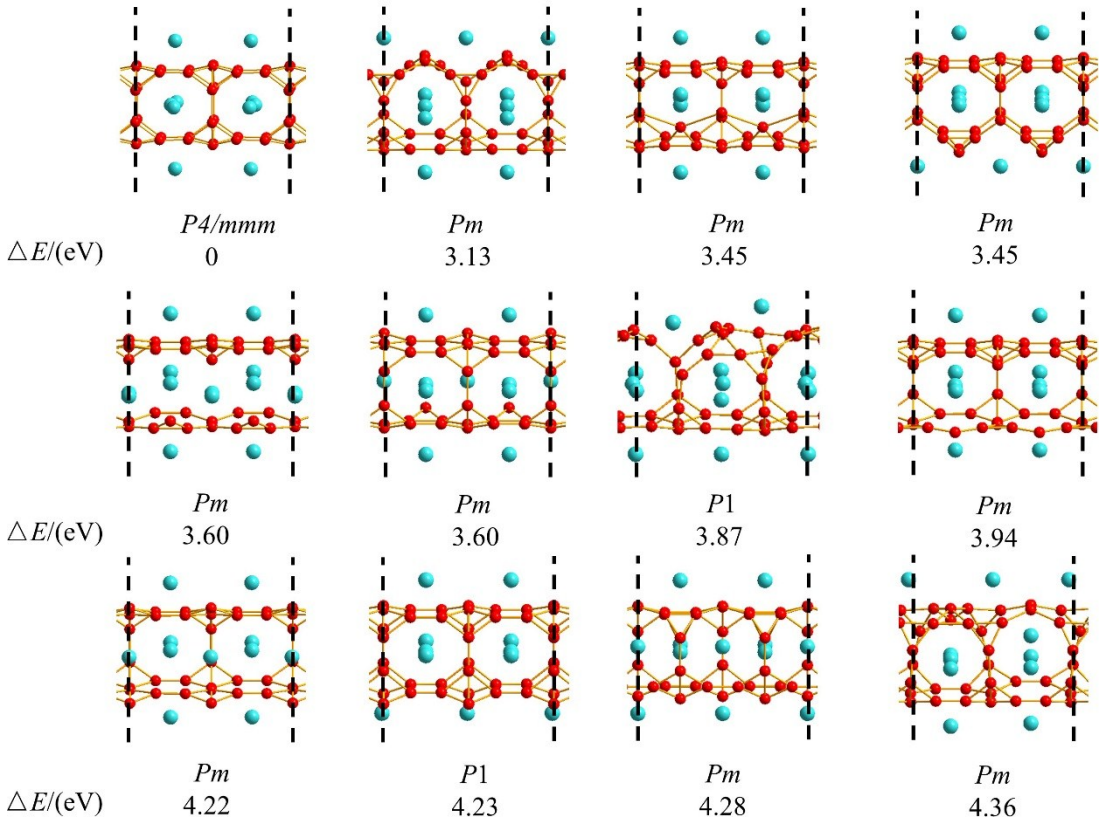


Fig. S5 Relative energies per unit cell (eV) of the low-lying isomers of 2D La_3B_{10} (**6**) nanosheet.

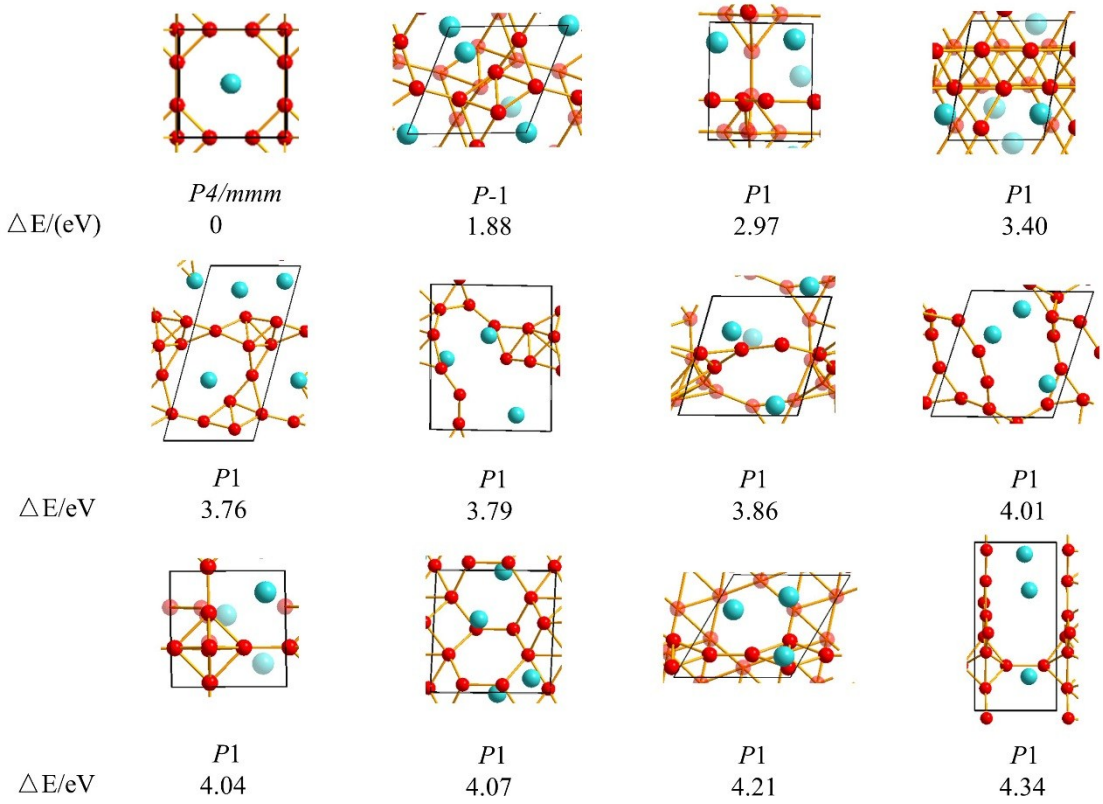


Fig. S6. Molecular orbital energy levels of O_h La_6&$[La@B_{24}]^+$ (**3**) at PBE0, with the pictures of the frontier orbitals HOMO-2 (t_{2g}), HOMO-1 (a_{2u}), HOMO (e_g), LUMO (a_{2g}), and LUMO+1 (t_{2u}) depicted.

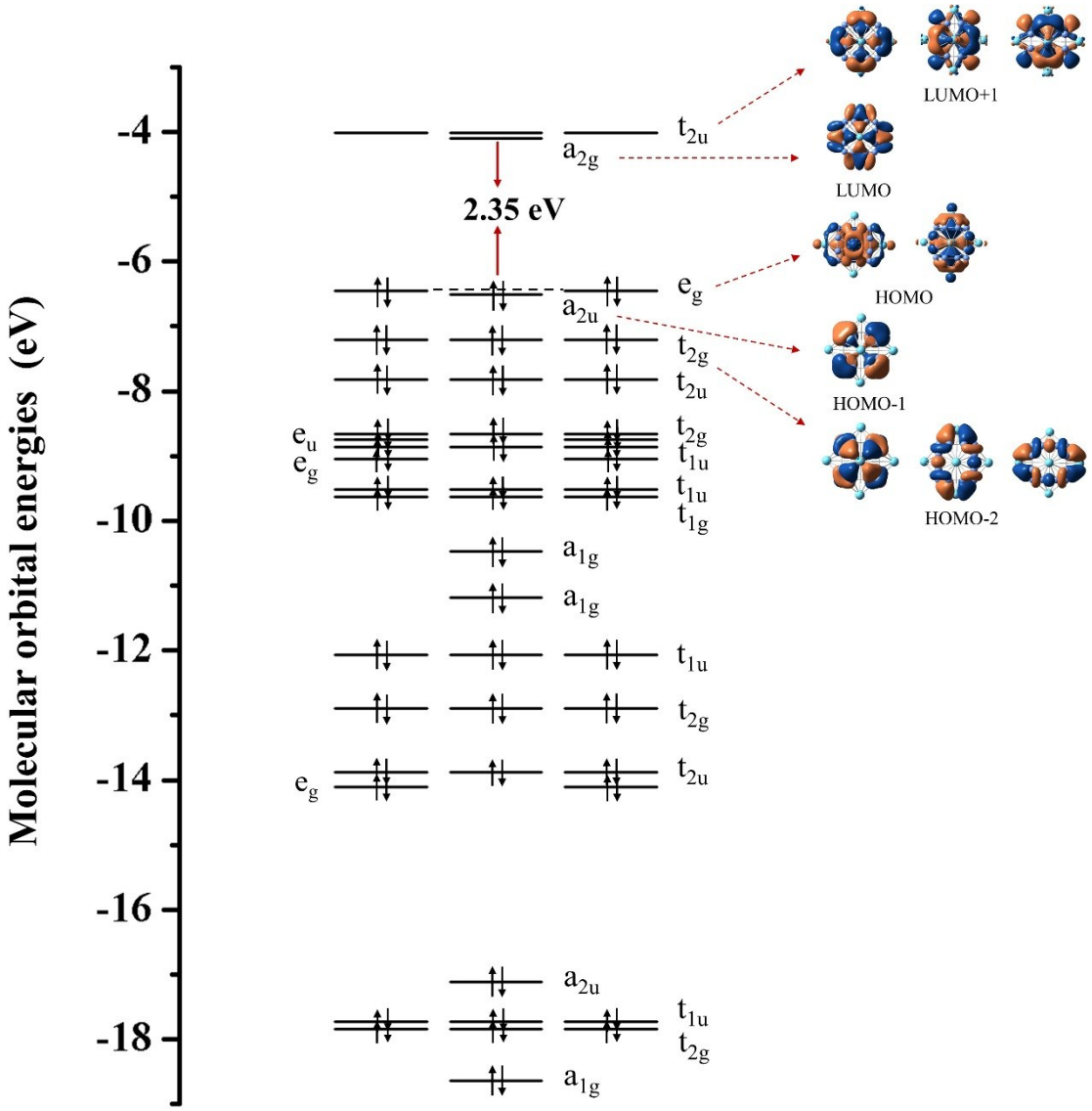


Fig. S7. AdNDP bonding analysis of O_h La_6&$[La@B_{24}]^+$.

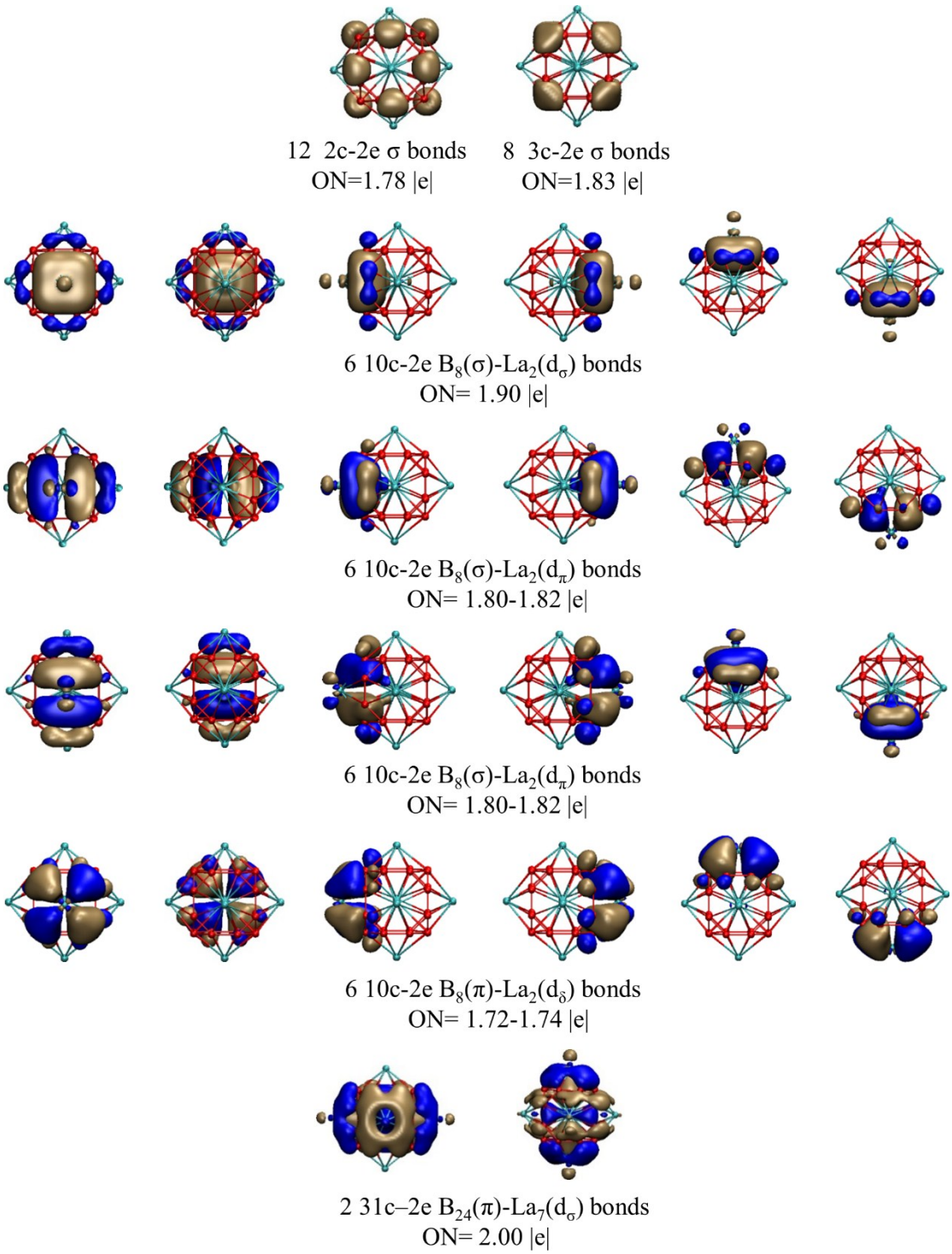


Fig. S8. IR and Raman spectra of O_h La_6&[La@B_{24}] (**4**) at PBE0/6-31G level.

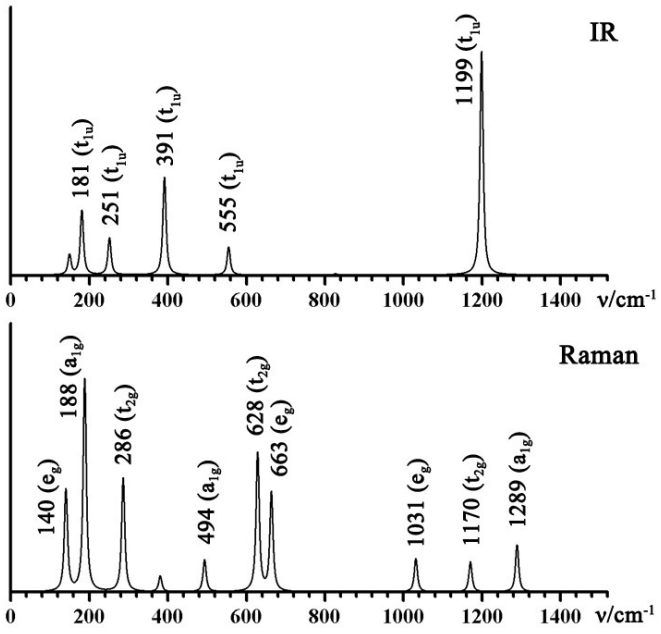


Table S1. Optimized coordinates (x, y, z) of O_h La_6&$[La@B_{24}]^+$ (**3**) at PBE0 level.

O_h La_6&$[La@B_{24}]^+$ (**3**)

B	0.83598000	1.99439600	1.99439600
B	1.99439600	1.99439600	0.83598000
B	1.99439600	1.99439600	-0.83598000
B	0.83598000	1.99439600	-1.99439600
B	-0.83598000	1.99439600	-1.99439600
B	-0.83598000	1.99439600	1.99439600
B	1.99439600	-0.83598000	1.99439600
B	1.99439600	-0.83598000	-1.99439600
B	1.99439600	0.83598000	-1.99439600
B	1.99439600	0.83598000	1.99439600
B	-1.99439600	1.99439600	0.83598000
B	-1.99439600	1.99439600	-0.83598000
B	-1.99439600	0.83598000	-1.99439600
B	-1.99439600	-0.83598000	-1.99439600
B	-1.99439600	-1.99439600	-0.83598000
B	-1.99439600	-1.99439600	0.83598000
B	-1.99439600	-0.83598000	1.99439600
B	-1.99439600	0.83598000	1.99439600
B	0.83598000	-1.99439600	-1.99439600
B	-0.83598000	-1.99439600	-1.99439600
B	-0.83598000	-1.99439600	1.99439600
B	0.83598000	-1.99439600	1.99439600
B	1.99439600	-1.99439600	0.83598000
B	1.99439600	-1.99439600	-0.83598000
La	0.00000000	0.00000000	0.00000000
La	0.00000000	3.61771000	0.00000000
La	-3.61771000	0.00000000	0.00000000
La	0.00000000	-3.61771000	0.00000000
La	3.61771000	0.00000000	0.00000000
La	0.00000000	0.00000000	-3.61771000
La	0.00000000	0.00000000	3.61771000

O_h La_6&[La@B_{24}] (**4**)

B	0.83529900	2.00166200	2.00166200
B	2.00166200	2.00166200	0.83529900
B	2.00166200	2.00166200	-0.83529900
B	0.83529900	2.00166200	-2.00166200
B	-0.83529900	2.00166200	-2.00166200
B	-0.83529900	2.00166200	2.00166200
B	2.00166200	-0.83529900	2.00166200
B	2.00166200	-0.83529900	-2.00166200
B	2.00166200	0.83529900	-2.00166200
B	2.00166200	0.83529900	2.00166200
B	-2.00166200	2.00166200	0.83529900
B	-2.00166200	2.00166200	-0.83529900
B	-2.00166200	0.83529900	-2.00166200
B	-2.00166200	-0.83529900	-2.00166200
B	-2.00166200	-2.00166200	-0.83529900
B	-2.00166200	-2.00166200	0.83529900
B	-2.00166200	-0.83529900	2.00166200
B	-2.00166200	0.83529900	2.00166200
B	0.83529900	-2.00166200	-2.00166200
B	-0.83529900	-2.00166200	-2.00166200
B	-0.83529900	-2.00166200	2.00166200
B	0.83529900	-2.00166200	2.00166200
B	2.00166200	-2.00166200	0.83529900
B	2.00166200	-2.00166200	-0.83529900
La	0.00000000	0.00000000	0.00000000
La	0.00000000	3.59694800	0.00000000
La	-3.59694800	0.00000000	0.00000000
La	0.00000000	-3.59694800	0.00000000
La	3.59694800	0.00000000	0.00000000
La	0.00000000	0.00000000	-3.59694800
La	0.00000000	0.00000000	3.59694800

Table S2. Optimized coordinates (x, y, z) of 1D $La_{10}B_{32}$ (**5**) nanowire, 2D La_3B_{10} (**6**) nanosheet and 3D LaB_6 (**7**) nanocrystal.

1D $La_{10}B_{32}$ (**5**) nanowire

8.6599387	-0.0000144	0.0000376
0.0002466	20.0466895	0.0002369
0.0005810	0.0001674	20.0415821

B	La
32	10

B	0.347812757	0.641005914	0.618187596
B	0.848917369	0.641987136	0.619173471
B	0.34782079	0.641007549	0.429714584
B	0.848934676	0.641993393	0.428738814
B	0.162093742	0.642031628	0.428696203
B	0.663248026	0.640918468	0.429811965
B	0.16208751	0.642024749	0.619213845
B	0.663236806	0.640913035	0.618095237
B	0.005562204	0.655843798	0.568655736
B	0.505468945	0.657780805	0.570304728
B	0.005564189	0.655847571	0.479256864
B	0.505476427	0.657781767	0.477599713
B	0.005572438	0.591489439	0.414873646
B	0.505493334	0.593139365	0.412938135
B	0.005574664	0.502108332	0.414875159
B	0.505500594	0.500460667	0.412940984
B	0.005573769	0.437753039	0.479260995
B	0.505481753	0.435813239	0.477599659
B	0.005567591	0.43775074	0.568661842
B	0.505473414	0.435813806	0.570308938
B	0.005559332	0.502106268	0.633045056
B	0.505474123	0.50046003	0.634953537
B	0.005560389	0.591491685	0.633044849
B	0.505474898	0.59313535	0.634954369
B	0.34782639	0.452590397	0.429715418
B	0.848941475	0.451604343	0.428739595

B	0.162101936	0.451567257	0.428698321
B	0.663253607	0.452678528	0.429813036
B	0.162094059	0.451570098	0.619217553
B	0.663238573	0.45268356	0.618099851
B	0.347813872	0.452590017	0.618190129
B	0.848921472	0.451609629	0.619179333
La	0.230512283	0.546798465	0.52395294
La	0.781472898	0.546797746	0.523954489
La	0.258576122	0.727300178	0.523951892
La	0.752441598	0.727269491	0.523956861
La	0.258582713	0.366299972	0.523956388
La	0.752450526	0.366328492	0.523960991
La	0.258587439	0.546803155	0.343407297
La	0.752468033	0.546802498	0.343440785
La	0.258580574	0.546796577	0.704503863
La	0.752426672	0.546801829	0.704475303

2D La_3B_{10} (**6**) nanosheet

4.174104434	0.0000000	0.0000000
0.0000000	4.1741084	0.0000000
0.0000000	0.0000000	20.4271340

B	La
10	3

B	0.687227	0.004261	0.604043
B	0.987522	0.004261	0.543386
B	0.28782	0.004261	0.604043
B	0.987523	0.304559	0.604043
B	0.987526	0.30457	0.401715
B	0.987526	0.703978	0.401714
B	0.987523	0.703965	0.604043
B	0.687231	0.004273	0.401714
B	0.287823	0.004273	0.401715
B	0.987525	0.00427	0.462371
La	0.487492	0.504223	0.502883
La	0.487526	0.504272	0.322547
La	0.487526	0.504264	0.683213

3D LaB_6 (**7**) nanocrystal

4.1630620	0.0000002	0.0000002
0.0000002	4.1630640	0.0000001
0.0000002	0.0000001	4.1630639

B La
6 1

B	0.706579	0.981909	0.998719
B	0.00648	0.981909	0.698819
B	0.00648	0.981909	0.298619
B	0.30638	0.981909	0.998719
B	0.00648	0.281809	0.998719
B	0.00648	0.682009	0.998719
La	0.506482	0.481925	0.498734