Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Material

B_{96}: A Complete Core-Shell Structure with High Symmetry

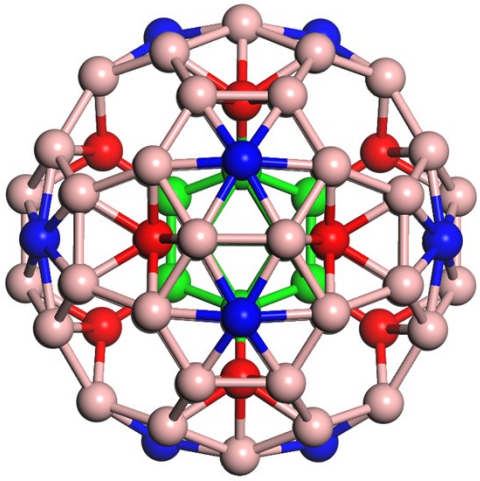
Linwei Sai[a], Xue Wu[b], Fengyu Li[c,*]

[a] *School of Science, Hohai University, Changzhou 213022, China*

[b] *State Key Laboratory of Metastable Materials Science and Technology and Key Laboratory for Microstructural Material Physics of Hebei Province, School of Science, Yanshan University, Qinhuangdao 066004, China*

[c] *School of Physical Science and Technology, Inner Mongolia University, Hohhot, 010021, China*

*Corresponding Author: fengyuli@imu.edu.cn



T_h B_{96} 5.749 eV/atom

Fig. S1 The T_h B_{96} isomer with concave penta-pyramids. Atoms highlighted in red, blue and green are pentagon capped B, hexagon capped B and core B, respectively.

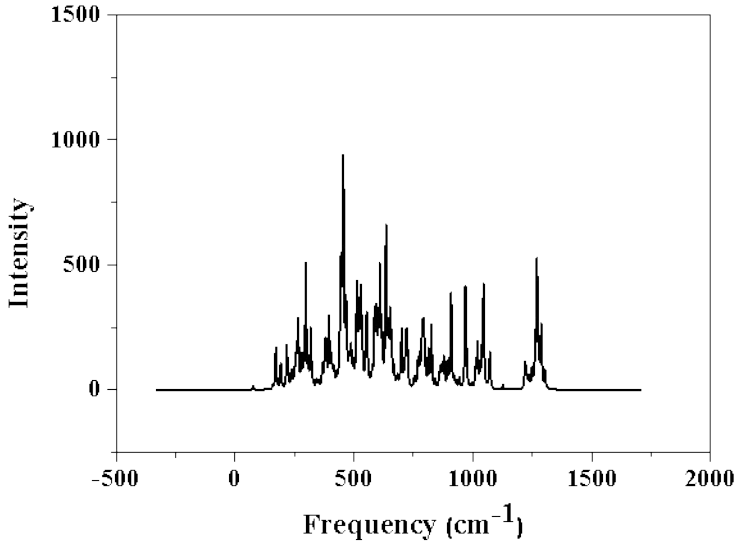


Fig. S2 The computed vibrational frequencies of T_h B_{96}.

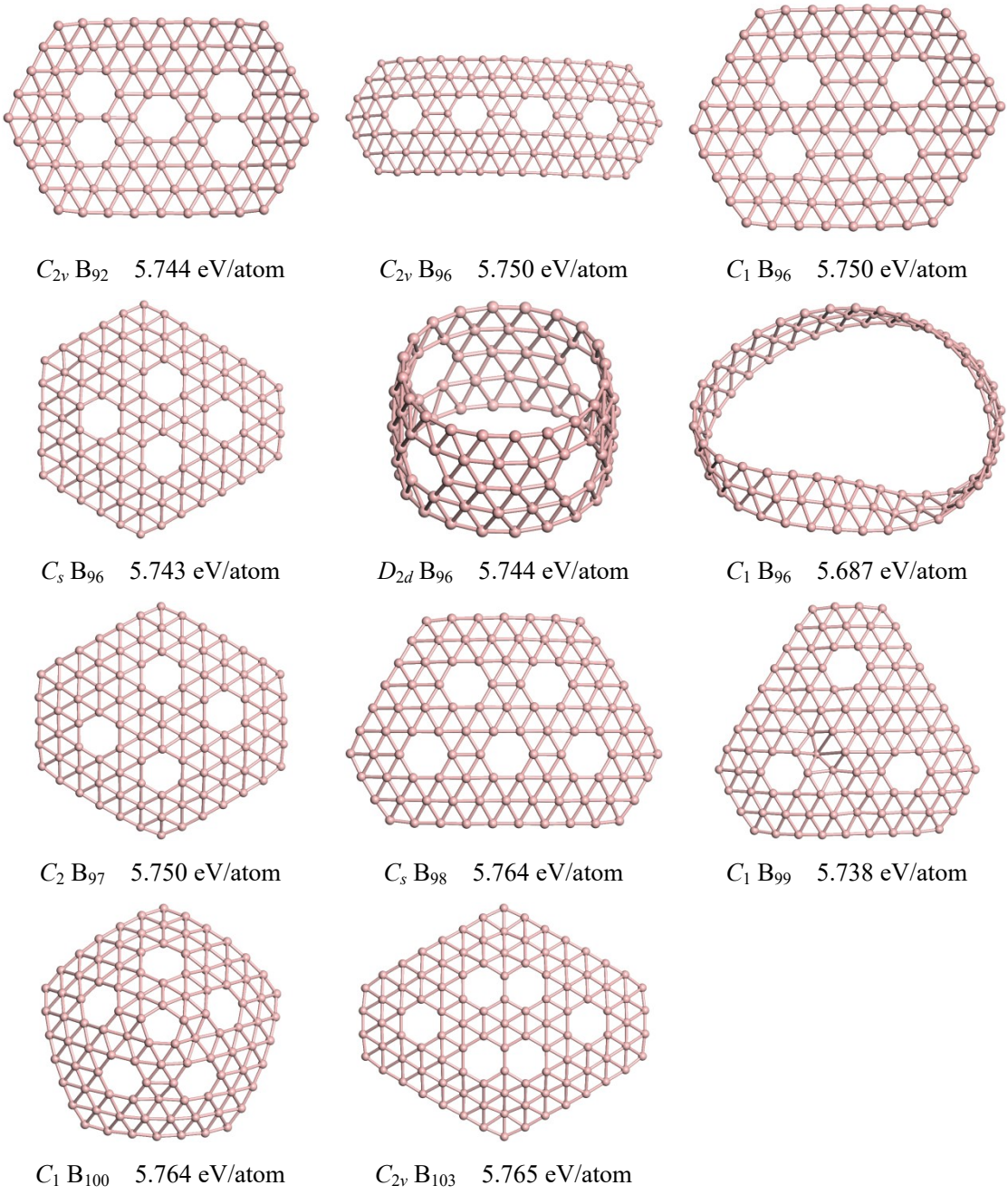


Fig. S3 Structures and cohesive energies of B_n clusters near size n = 96 of the planar, ring and Möbius ring configurations at the PBE/DND level of theory.

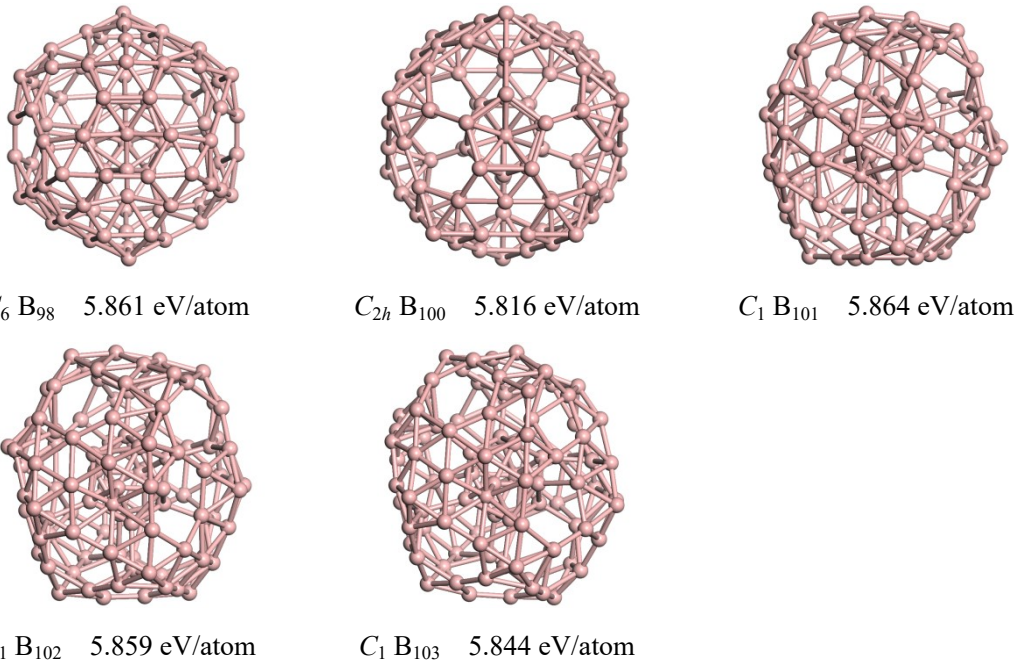


Fig. S4 Structures and cohesive energies of core-shell boron clusters from Ref.S1 and Ref.S2 at the PBE/DND level of theory.

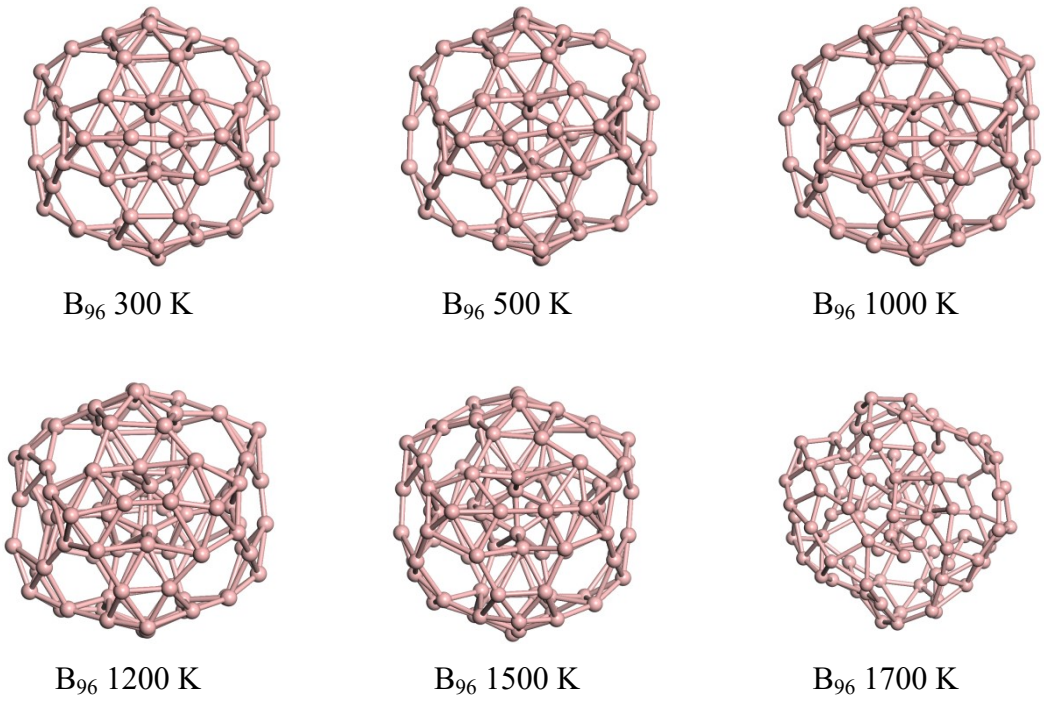


Fig. S5 The final structures of T_h B_{96} through 5 ps's first-principles molecular dynamics simulations at temperature 300, 500, 1000, 1200, 1500 and 1700 K, respectively.

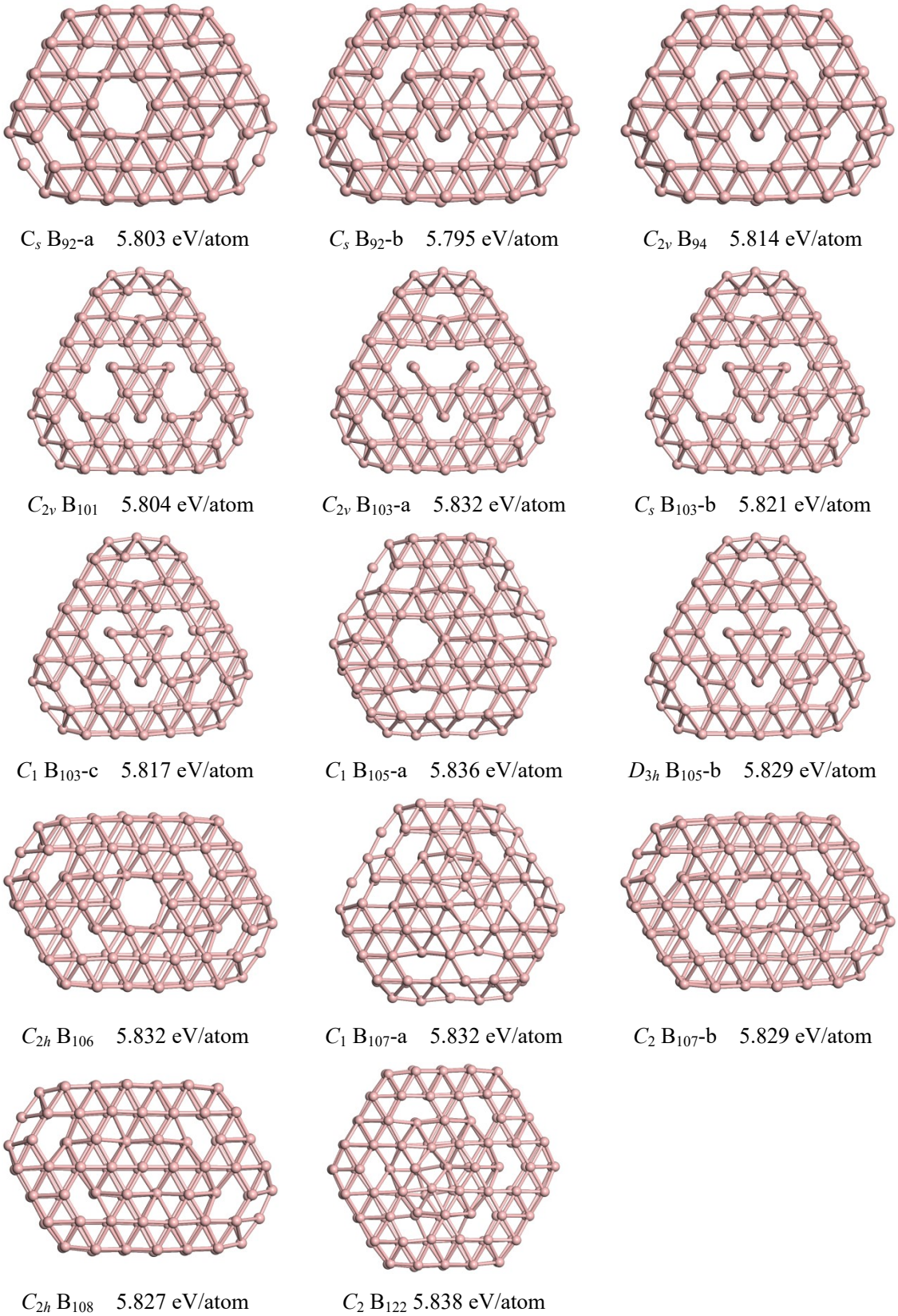


Fig. S6 Structures and cohesive energies of bilayer boron clusters at the PBE/DND level of theory.

Table S1 The optimized coordinates of T_h B_{96} at TPSSh/6-311G(d) level.

B	3.225461	0.88792	2.816498
B	-0.81408	1.89E-05	4.226666
B	0.814087	2.23E-05	4.226654
B	-1.68326	-1.43653	3.602799
B	-1.43658	3.602911	1.683268
B	-0.8879	2.816469	3.225321
B	1.683261	1.436507	3.602672
B	-1.68325	1.436502	3.602676
B	0.887896	2.816472	3.225329
B	3.602826	1.683262	1.436533
B	-3.60279	-1.68328	-1.43652
B	-3.22539	-0.88796	-2.8165
B	3.225444	0.887916	-2.81648
B	-1.43652	-3.60279	1.683262
B	-0.88792	2.816477	-3.22533
B	3.602805	1.68326	-1.43652
B	-2.81649	-3.2254	0.887923
B	-1.68325	1.436511	-3.6027
B	1.68326	1.436515	-3.60268
B	-0.88794	-2.81651	3.225416
B	0.887907	2.816478	-3.22533
B	2.816487	-3.22542	-0.88792
B	1.436527	-3.6028	-1.68327
B	-2.81659	3.225475	0.887999
B	3.602787	-1.68328	-1.43652
B	9.97E-06	-4.22671	-0.81409
B	-2.81659	3.225474	-0.88799
B	4.226697	0.814079	8.91E-06
B	-2.81648	-3.22541	-0.88793
B	-3.22542	0.887925	-2.81648
B	3.225399	-0.88796	-2.81651
B	7.8E-06	-4.22672	0.814085
B	-1.43657	3.602882	-1.68326
B	4.226707	-0.8141	7.47E-06
B	-1.43651	-3.6028	-1.68327
B	-3.6028	1.683264	-1.43651
B	0.814082	2.13E-05	-4.22663
B	-0.81408	1.45E-05	-4.22664
B	0.887967	-2.81654	-3.22543
B	-1.68326	-1.43655	-3.60283
B	1.683268	-1.43655	-3.60284
B	-0.88797	-2.81654	-3.22543
B	-3.22542	-0.88797	2.816508
B	1.436577	3.602887	-1.68327
B	0.887948	-2.81651	3.225417
B	-3.60283	-1.68328	1.436532
B	2.816579	3.225468	-0.88799
B	1.683268	-1.43653	3.602803
B	-3.60282	1.68326	1.436525

B	1.08E-05	4.226701	0.814072
B	2.816487	-3.2254	0.887921
B	-4.22672	-0.8141	5.69E-06
B	2.816577	3.225463	0.887986
B	3.225432	-0.88796	2.81652
B	-3.22545	0.887921	2.816488
B	9.72E-06	4.226685	-0.81407
B	1.436522	-3.6028	1.683265
B	-4.2267	0.814079	7.71E-06
B	1.436575	3.602902	1.683267
B	3.602829	-1.68328	1.436541
B	0.853656	-1.42543	-2.1E-06
B	-0.85367	-1.42546	1.92E-06
B	-1.7E-05	-0.85373	1.425483
B	1.425472	-5.8E-05	0.853768
B	-1.42545	-4.1E-05	-0.85373
B	-0.8541	1.425504	6.5E-06
B	0.854106	1.425453	6.96E-07
B	-2.3E-05	-0.85378	-1.4255
B	-9E-06	0.853784	1.425208
B	1.425434	-5.4E-05	-0.85379
B	-2E-05	0.853843	-1.42522
B	-1.42548	-4.2E-05	0.853723
B	-3.07329	-1.8E-05	-1.28992
B	-1.29005	3.073391	1.13E-05
B	-3.0733	-3.2E-05	1.289934
B	-5E-07	1.289891	-3.07309
B	3.58E-06	-1.28994	3.073319
B	1.29005	3.073334	-8.7E-07
B	-1.2899	-3.0733	1.03E-06
B	1.289896	-3.07326	6.78E-07
B	8.26E-07	-1.28998	-3.07333
B	3.073305	-2.9E-05	1.289944
B	3.073282	-1.9E-05	-1.28993
B	1.5E-06	1.28987	3.073081
B	-1.2E-06	3.958636	-2.46859
B	1.67E-06	3.958645	2.468592
B	-3.95864	2.46863	3.57E-06
B	-2.46861	3.61E-06	-3.9586
B	2.468617	7.9E-06	-3.9586
B	3.95862	-2.46863	-3.5E-07
B	1.69E-06	-3.95863	2.468625
B	-3.95863	-2.46864	-5.7E-06
B	4.73E-06	-3.95863	-2.46863
B	3.95863	2.46862	6.32E-07
B	2.468624	8.49E-06	3.958604
B	-2.46861	5.17E-06	3.958586

References:

S1 D. L. V. K. Prasad and R. D. Jemmis, *Phys. Rev. Lett.*, 2008, **100**, 165504.

S2 F. Li, P. Jin, D.-E. Jiang, L. Wang, S. B. Zhang, J. Zhao and Z. Chen, *J. Chem. Phys.*, 2012, **136**, 074302.