Electronic Supplementary Material (ESI) for Nanoscale.

Electronic Supplementary Information

B_{28}: smallest all-boron cage from *ab initio* global search

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Table S1. Energy differences of the four presentative low-lying B_{28} cluster isomers shown in Figure 1 (neutral and anion) using PBE0 functional with different basis sets.

Clusters	Basis set	Energy differences (eV)			
		Cage	Quasi-planer	Tube	Bowl
B_{28}	cc-pVDZ	0	0.003	0.176	1.746
	aug-cc-pVDZ	0	0.133	0.340	1.832
	6-311+G(d)	0	0.034	0.173	1.766
	6-311+G(3df,2p)	0	0.012	0.245	1.765
B_{28}^-	cc-pVDZ	0	0.130	0.174	1.471
	aug-cc-pVDZ	0	0.282	0.321	1.538
	6-311+G(d)	0	0.182	0.112	1.461
	6-311+G(3df,2p)	0	0.150	0.171	1.440

Table S2. Energy differences of the four presentative low-lying B_{28} cluster isomers shown in Figure 1 (neutral and anion) using PBE0 and PBE with 6-311+G(d) basis set.

Clusters	Functionals	Energy differences (eV)			
		Cage	Quasi-planer	Tube	Bowl
B_{28}	PBE	0.070	0	0.264	1.659
	PBE0	0	0.034	0.173	1.766
B_{28}^-	PBE	0.050	0	0.126	1.235
	PBE0	0	0.182	0.112	1.461

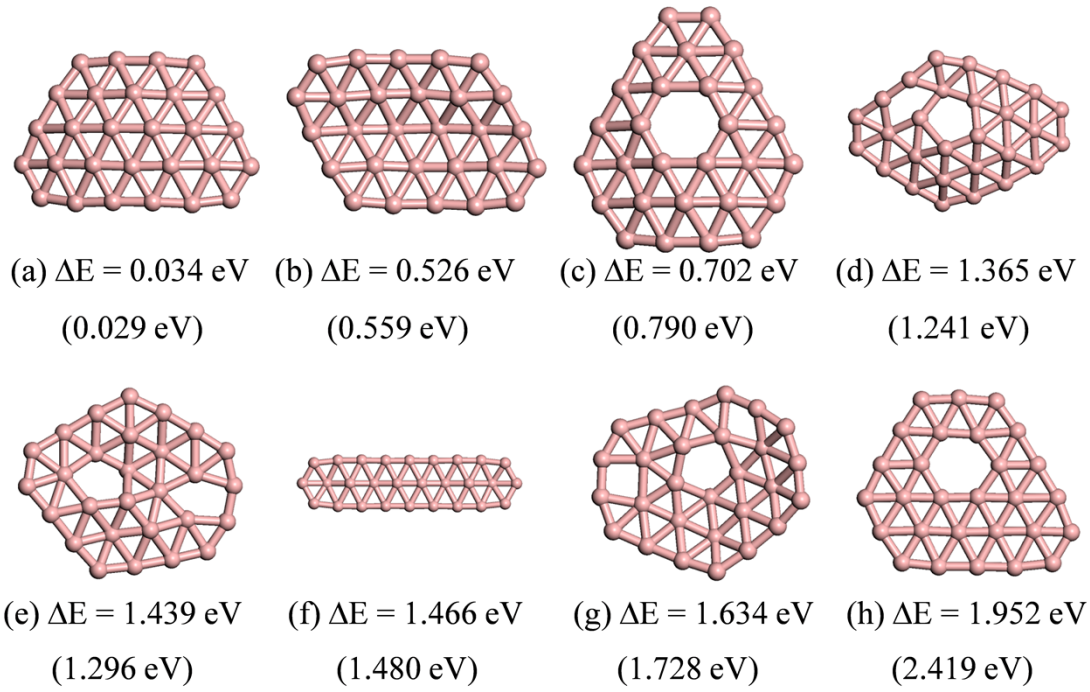

Figure S1. Planar and quasi-planar isomer structures of B_{28}. For each isomer, the relative energy (ΔE) to the ground state cage structure at PBE0/6-311+G(d) level is given. The single-point energy results of CCSD(T)/def2-TZVP calculations are provided in parenthesis.

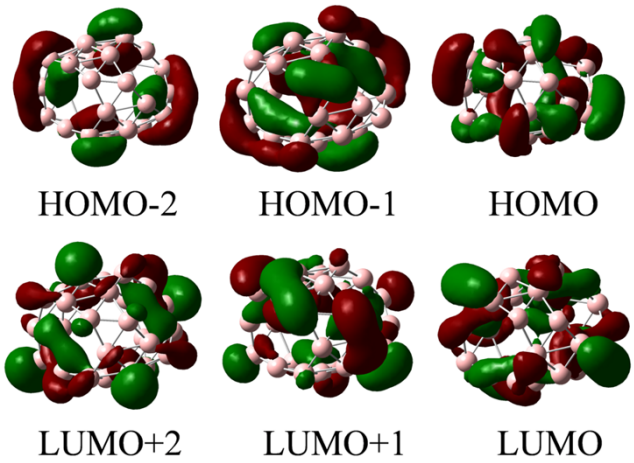

Figure S2. Spatial distributions of HOMO−2, HOMO−1, HOMO, LUMO, LUMO+1, LUMO+2 molecule orbitals in the lowest-energy cage of B_{28}. Green and red denote the wavefunction of positive and negative phases, respectively.