Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

B_{40}: cluster stability, reactivity, and its planar structural precursor

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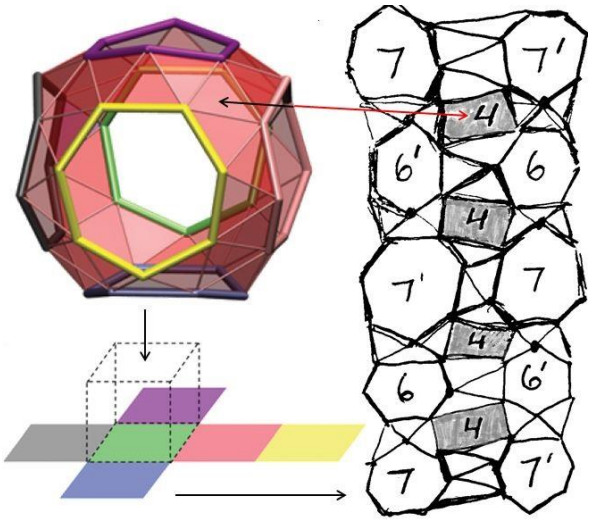

Figure S1. Unfolding a cube (bottom left) turns the triplets of the facets at each (of eight) vertices into quartets of coplanar squares, thus eliminating the vertex-disclinations. Accordingly, the eight triangular facets of B_{40}-polyhedron are transformed into rectangles, allowing one to sketch the planar lattice, on the right. Note that the heptagons 7 and 7' are inverted, while the hexagons 6 and 6' are 90-rotated.

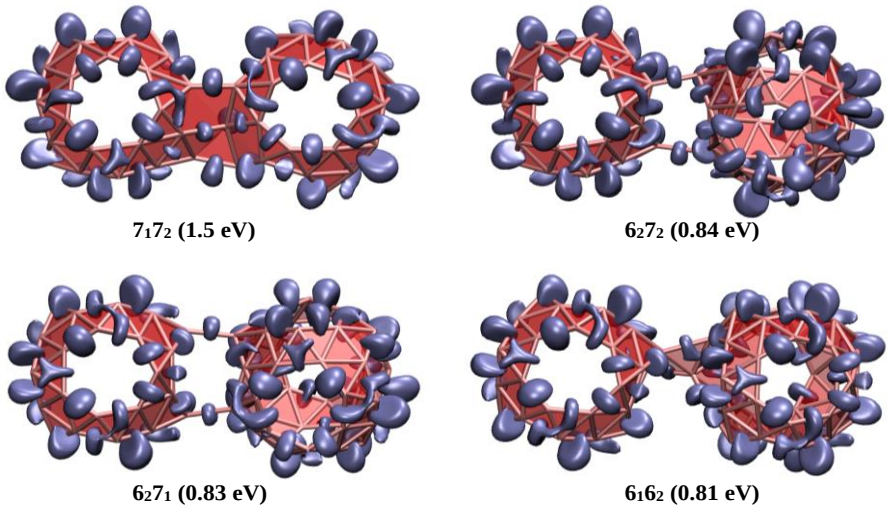

Figure S2. Four directions of interaction among eight with the largest binding energy according to the types of heptagons and hexagons using electron localization function.

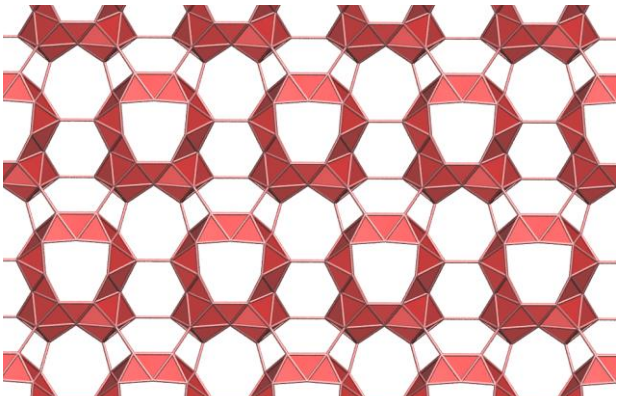

Figure S3. The orthographic view of fused 2D B_{40} cages.

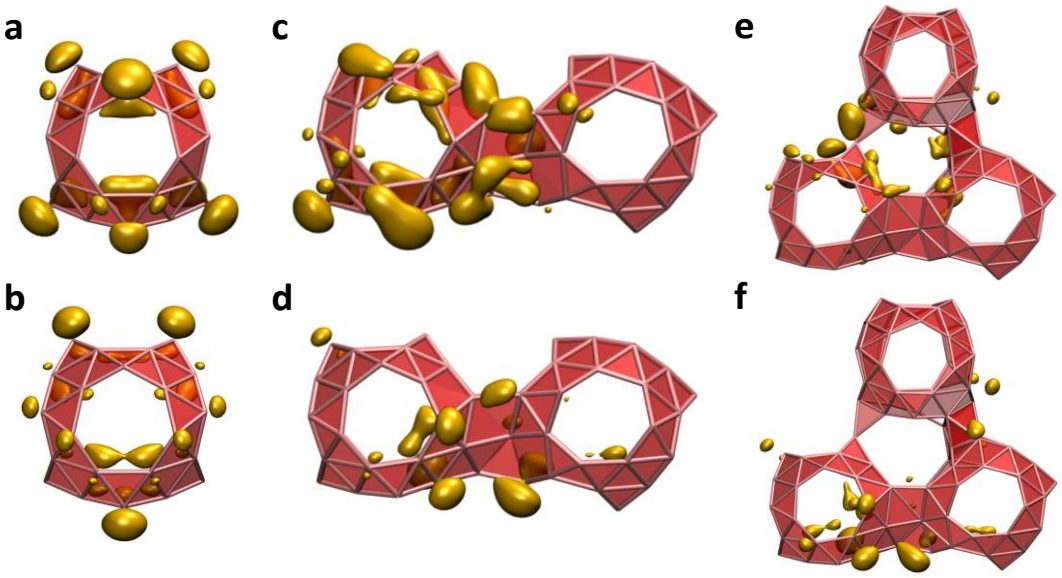

Figure S4. The HOMO and LUMO pictures of B_{40} single cage (a,b), dimer (c,d) and trimer (e,f) respectively.

Table S1. Number (N), average length (L) and energy (E_{bond}) of created bonds, binding energy of the B_{40} dimer (E_b) for 8 directions of interactions (D) in total, according to the types of heptagons and hexagons.

D	N	L (Å)	E_{bond} (eV)	E_b (eV)
$6_1 - 6_1$	2	1.96	0.68	0.44
$6_1 - 6_2$	2	1.89	0.85	0.81
$7_1 - 7_1$	3	1.87	0.89	0.68
$7_1 - 7_2$	5	1.74	1.20	1.50
$6_1 - 7_1$	2	1.84	0.96	0.64
$6_1 - 7_2$	2	1.84	0.97	0.65
$6_2 - 7_1$	2	1.86	0.94	0.83
$6_2 - 7_2$	2	1.86	0.96	0.85