Supporting information for

B_{92}: a complete coating icosahedral B_{12} core-shell structure

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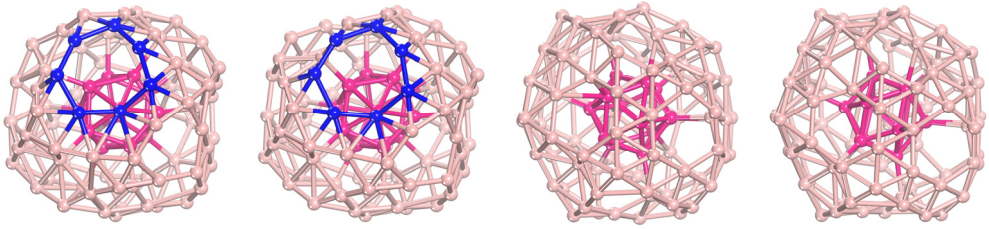
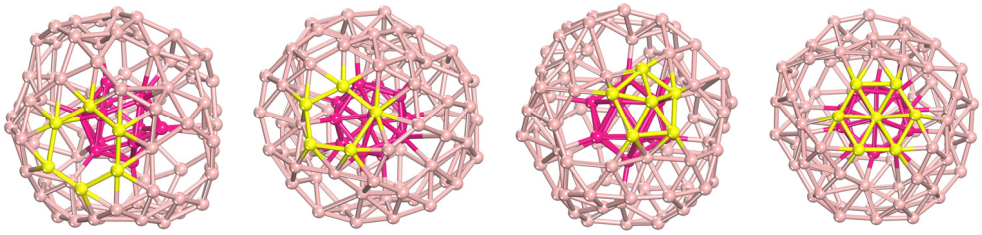


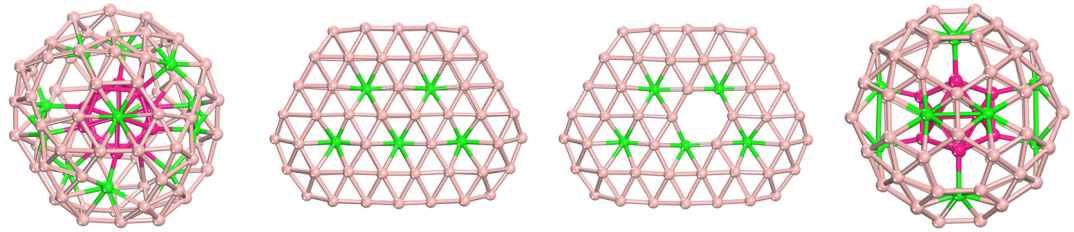
(*a*) (*b*) (*c*) (*d*)

Fig. S1 The PBE/DNP optimized structures: (*a*) $B_{12}@B_{78}$, (*b*) $B_{12}@B_{79}$, (*c*) $B_{12}@B_{81}$ and (*d*) $B_{12}@B_{82}$. The interior B_{12} icosahedron in the core-shell clusters and hollow heptagon are highlighted in magenta and blue, respectively.

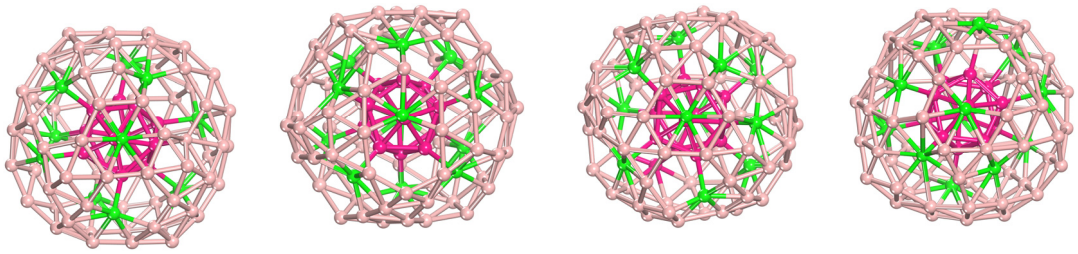


(*a*) (*b*) (*c*) (*d*)

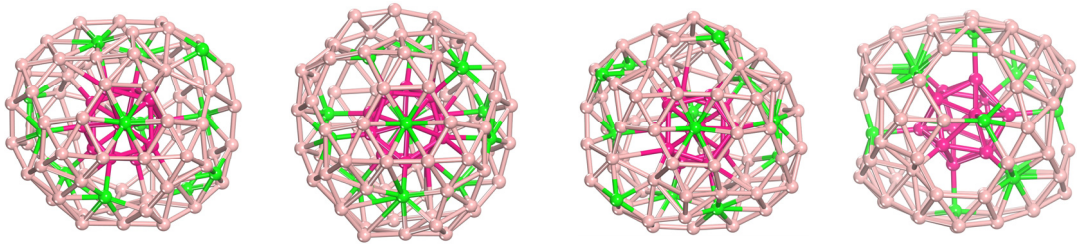
Fig. S2 The structural unit of the outer shell for $B_{12}@B_{80}$: (*a*) hollow hexagon, (*b*) hollow pentagon, (*c*) centered pentagons and (*d*) centered hexagons.



I-C_1 0.00 eV	II-C_s -1.38 eV	III-C_s -0.62 eV	IV-T_h -1.12 eV



V-C_i -0.29 eV	VI- C_i -0.71 eV	VII- C_1 -3.70 eV	VIII- C_1 -1.17 eV



IX- C_1 -0.22 eV	X- C_1 -0.53 eV	XI- C_1 -0.07 eV	XII- C_i -2.69 eV

Fig. S3 The optimized B_{92} isomers at the PBE/DNP level, with the relative binding energies (in eV) listed below. Here, the relative energy (ΔE) is relative to the core-shell I-C_1 B_{12}@B_{80} structure we studied, which is calculated as follows: E_b=E(B_{12}@B_{80})-92*E(B), ΔE=E_b(*isomer*)-E_b(I-C_1 B_{12}@B_{80}). A typical B_{92} isomer was the highly symmetrical IV-T_h B_{12}@B_{80} structure, which was constructed based on C_{60} fullerenes. 20 B atoms are added to the center of 20 hexagons of B_{60}. Among them, 12 B atoms are slightly concave inward and bond with the internal B_{12} icosahedron. These 12 inward-concave boron atoms are in the same position as the 12 slightly inward-concave B atoms in T_h B_{96}. The calculated results show that the binding energies of T_h B_{12}@B_{80} is 1.12 eV lower than that of the I-C_1 B_{12}@B_{80} structure we studied.

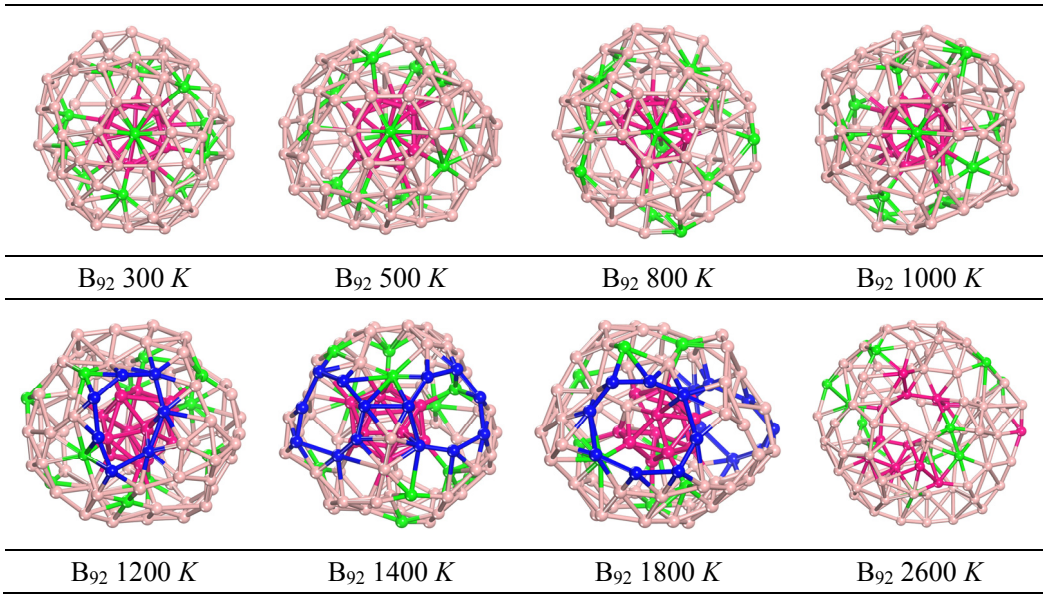


Fig. S4 The structures of the core-shell $B_{12}@B_{80}$ at temperature 300, 500, 800, 1000, 1200, 1400, 1800, and 2600 *K*, respectively.

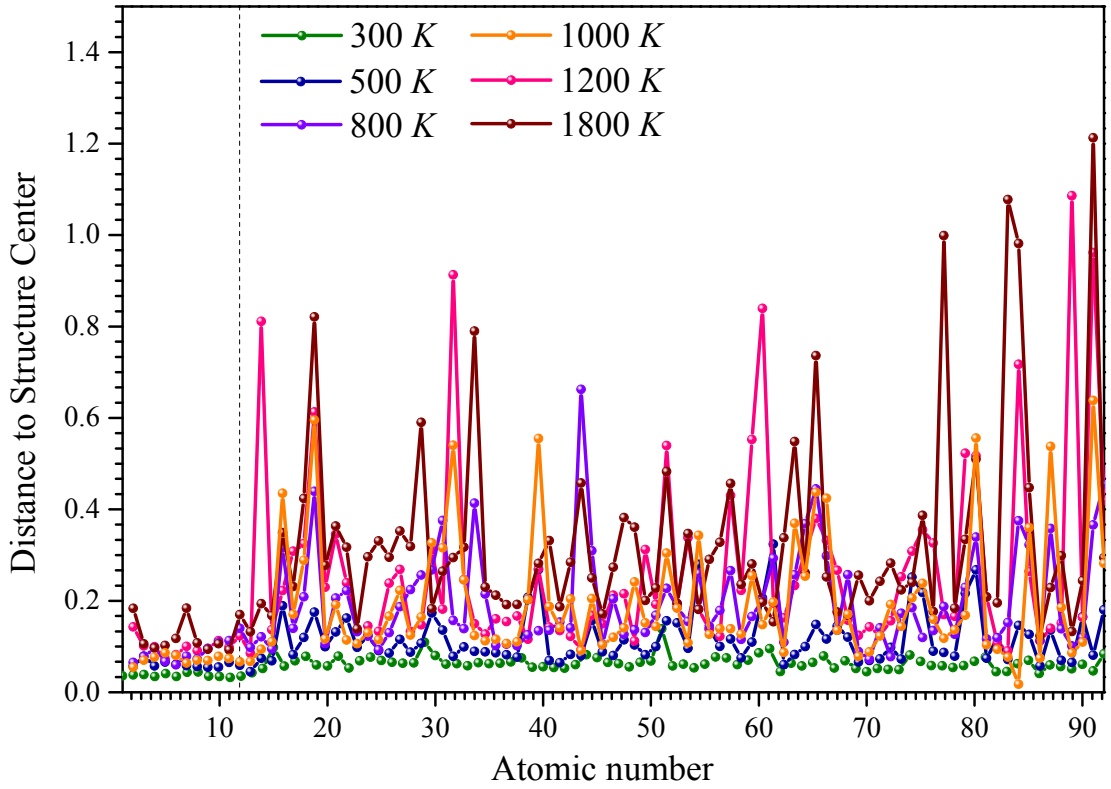


Fig. S5 The average displacement of individual atoms relative to the center of the $B_{12}@B_{80}$ system for various temperatures. The B_{12} core atoms in the $B_{12}@B_{80}$ structure are numbered 1 to 12, while atoms 13 to 92 correspond to the B_{80} shell. The left side of the dashed black line corresponds to the average displacement curve of the core atoms, while the right side indicates the average displacement curve of the shell atoms.

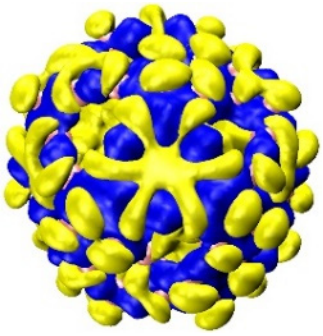


Fig. S6 Deformation electron density of $B_{12}@B_{80}$ structure, with the isovalue of 0.006 e/Å^3.

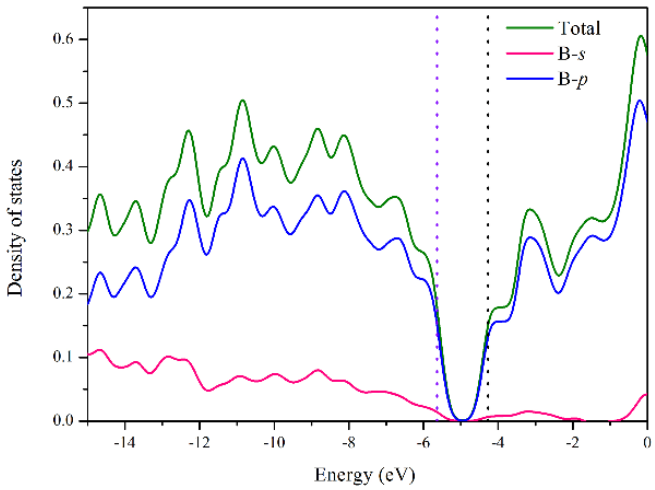


Fig. S7 The total and partial density of states of $B_{12}@B_{80}$ structure. The HOMO (purple) and LUMO (black) levels are shown by dashed lines.

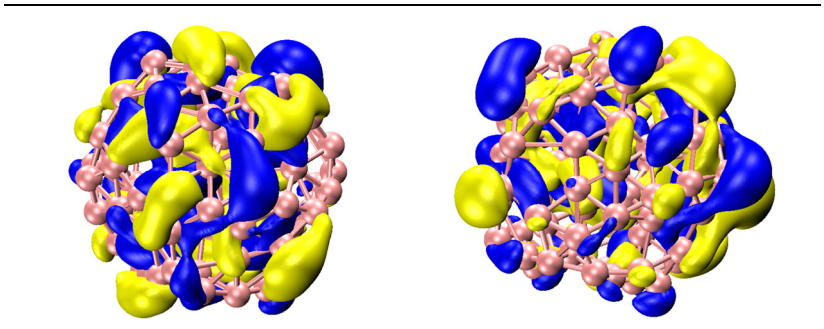


Fig. S8 HOMO and LUMO frontier molecular orbitals for the core-shell $B_{12}@B_{80}$ structure, with an isosurface of 0.015 e/Å^3.

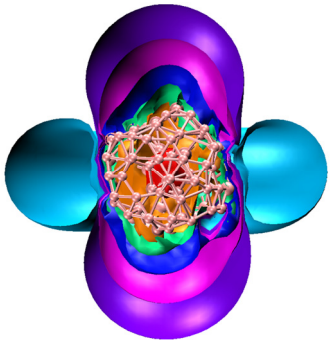


Fig. S9 ICSS_ZZ of the core-shell $B_{12}@B_{80}$ structure at different isosurfaces. Color scheme: red 64 ppm shielding, orange 32 ppm shielding, green 16 ppm shielding, blue 8 ppm shielding, magenta 4 ppm shielding, violet 2 ppm shielding, cyan -1.5 ppm deshielding for $B_{12}@B_{80}$ structure (note that the ICSS and NICS values are opposite in sign).

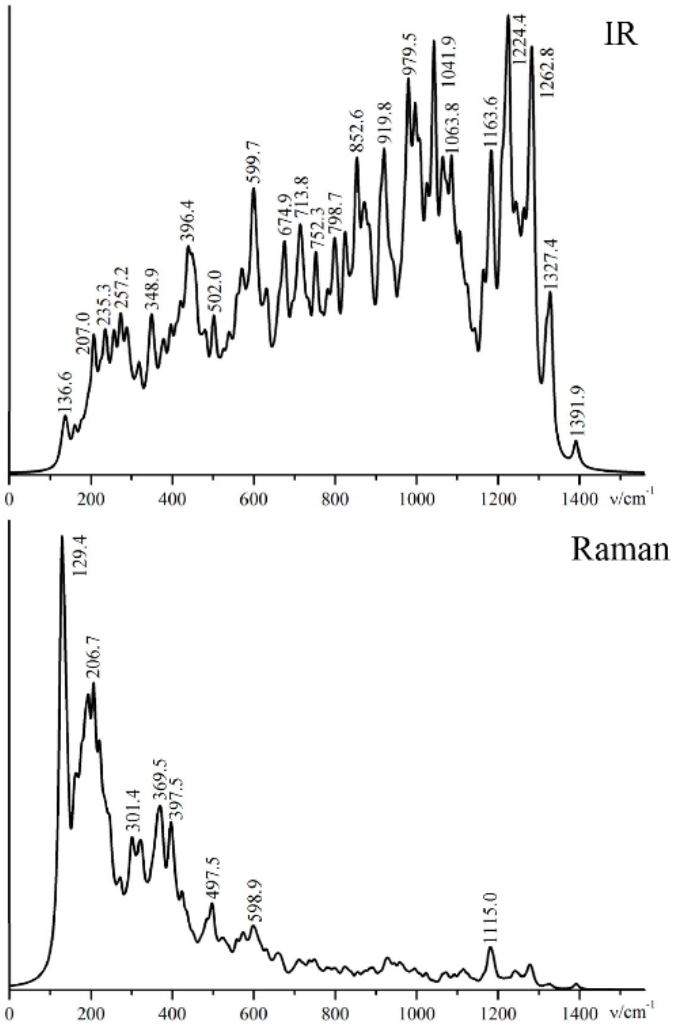


Fig. S10 Simulated IR and Raman spectrum of $B_{12}@B_{80}$ structure. For Raman spectrum, the incident light and incident temperature are set to 488 nm and 300 *K*, respectively. The Lorentzian smearing is set to 30.00 cm^{-1}.

Table S1. Cartesian coordinates of the core-shell $B_{12}@B_{80}$ structure.

Atoms	Number	X	Y	Z	Atoms	Number	X	Y	Z
B	1	2.930	-0.443	1.605	B	47	3.321	-2.190	-0.746
B	2	3.198	-2.232	2.048	B	48	2.679	-2.672	-2.264
B	3	1.489	-2.270	2.536	B	49	1.328	-3.575	-2.355
B	4	0.569	-3.680	2.009	B	50	-0.241	-1.028	-3.151
B	5	-1.064	-3.440	1.824	B	51	1.349	-0.382	-3.698
B	6	-1.855	-3.045	0.290	B	52	2.670	-1.107	-3.103
B	7	-3.562	-2.688	0.459	B	53	4.070	0.958	2.135
B	8	-4.236	-1.905	-0.803	B	54	2.114	-3.409	1.375
B	9	-4.370	-0.200	-0.687	B	55	-2.700	-3.188	1.735
B	10	-2.941	0.442	-1.559	B	56	-3.803	-0.978	-2.063
B	11	-2.830	2.091	-1.923	B	57	-2.162	3.608	-1.850
B	12	-1.713	2.612	-3.062	B	58	2.687	3.324	-1.857
B	13	-0.548	3.572	-2.178	B	59	0.227	3.883	2.244
B	14	1.063	3.426	-2.013	B	60	-3.932	1.462	2.116
B	15	2.012	3.818	-0.470	B	61	0.013	-0.540	4.419
B	16	3.328	2.594	-0.416	B	62	-0.295	-3.761	-2.414
B	17	4.255	1.773	0.779	B	63	-0.132	0.565	-3.940
B	18	4.372	0.077	0.590	B	64	3.913	-1.557	-2.164
B	19	3.092	0.380	3.275	B	65	-0.19	-2.291	2.797
B	20	1.587	2.967	2.242	B	66	2.616	-1.232	3.221
B	21	1.211	4.061	0.952	B	67	-4.104	-1.074	0.746
B	22	-0.760	4.189	0.984	B	68	-2.851	-2.763	-1.243
B	23	-1.511	3.991	-0.422	B	69	-2.538	1.180	-3.348
B	24	-3.010	3.103	-0.494	B	70	0.061	1.945	-2.624
B	25	-3.597	2.403	0.835	B	71	1.961	2.526	0.657
B	26	-4.306	0.613	0.719	B	72	4.265	1.137	-0.751
B	27	-3.811	-0.197	2.125	B	73	1.688	1.499	3.189
B	28	-1.960	-2.487	2.986	B	74	-1.769	2.645	0.749
B	29	-1.209	-1.510	3.987	B	75	-2.239	-0.784	2.595
B	30	1.569	-0.077	3.975	B	76	4.045	-1.608	0.721
B	31	0.131	0.850	3.430	B	77	1.777	-2.922	-0.484
B	32	0.100	2.359	2.899	B	78	-1.854	-1.688	-3.421
B	33	-1.334	3.373	2.389	B	79	2.256	0.438	-2.384
B	34	-2.669	2.460	2.338	B	80	1.145	-1.999	-3.074
B	35	-2.732	0.835	3.124	B	81	1.317	0.085	-0.948
B	36	-1.442	0.176	3.923	B	82	-1.538	0.048	-0.639
B	37	1.112	-4.251	0.513	B	83	0.200	-1.162	1.358
B	38	0.481	-4.148	-1.003	B	84	0.150	0.557	1.599
B	39	-1.257	-3.552	-1.119	B	85	-1.320	-0.287	1.141
B	40	-1.821	-3.118	-2.614	B	86	0.914	1.297	0.251
B	41	-3.057	-0.399	-3.395	B	87	-0.856	-1.537	-0.026
B	42	-1.540	-0.188	-3.957	B	88	0.874	-1.474	-0.239
B	43	1.246	1.322	-3.915	B	89	-0.863	1.280	0.417
B	44	2.080	2.290	-2.992	B	90	1.541	-0.193	0.777
B	45	3.329	1.704	-1.923	B	91	-0.106	1.005	-1.174
B	46	4.450	-0.950	-0.759	B	92	-0.156	-0.743	-1.418