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


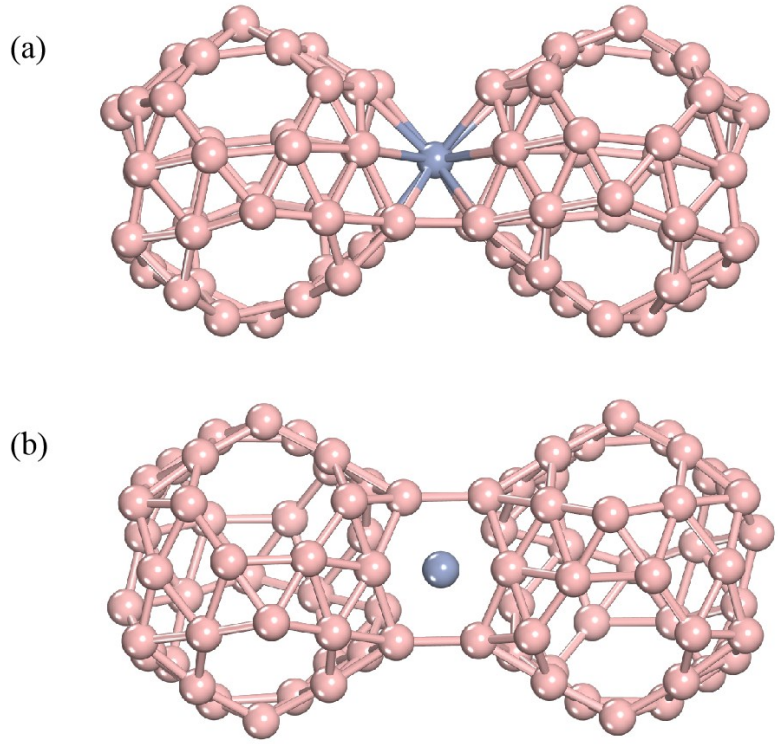


**Figure S1.** Optimized geometric structure of $7_3 \perp 7_1$ $B_{40}$ dimer intercalated by Cr atom (a) top view, (b) side view.

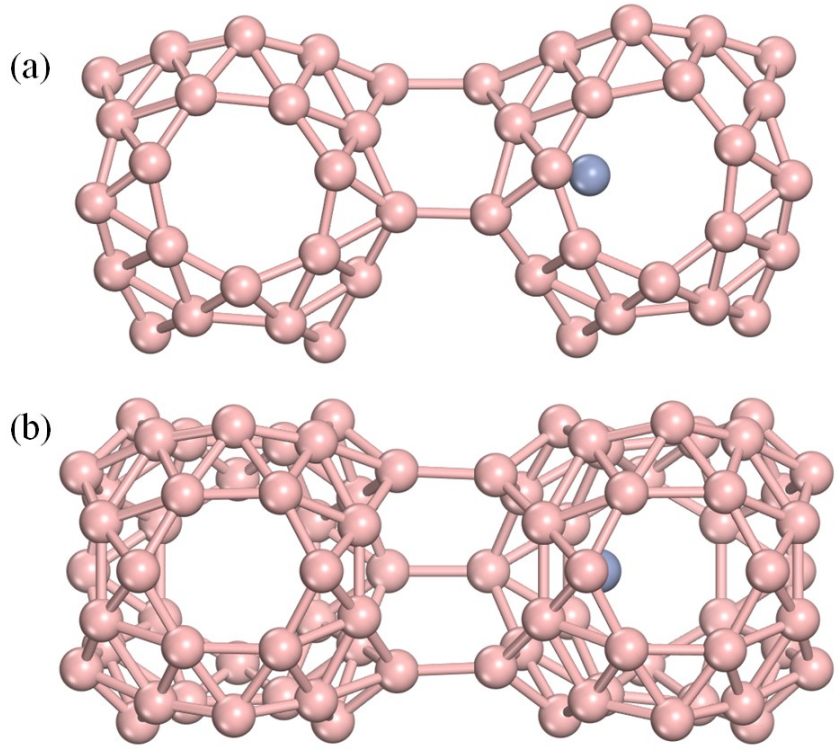


**Figure S2.** Optimized geometric structure of Cr-encapsulated $B_{40}CrB_{40}$ cluster (a) top view, (b) side view.

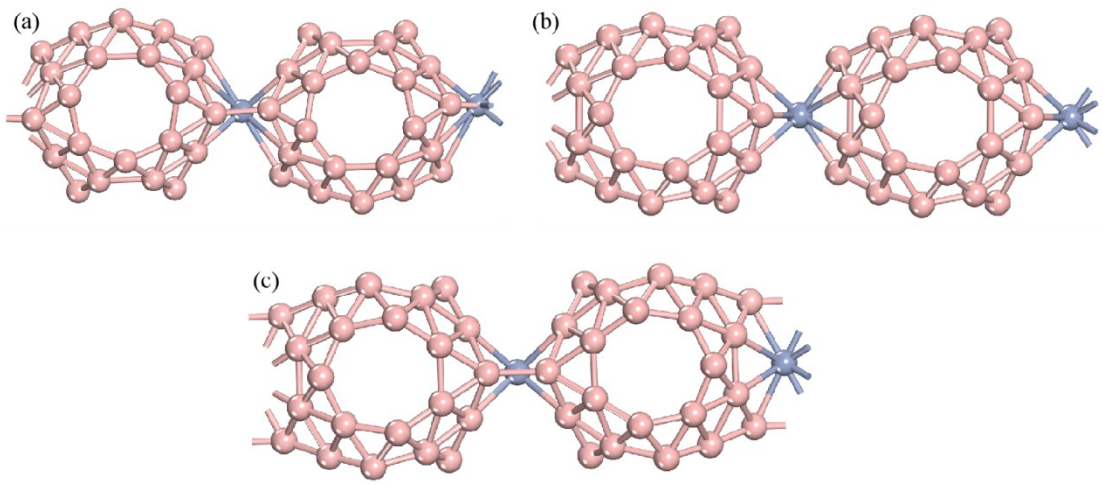


**Figure S3.** Optimized geometric structures of one-dimensional $B_{40}Cr$ polymer isomers (a) placing the heptagon of $B_{40}$ onto the antiparallel heptagon of another one with Cr located in the center; (b) stacking the hexagon of $B_{40}$ onto the vertical hexagon of another with Cr lying in the center; (c) stacking the hexagon of $B_{40}$ onto the parallel hexagon of another with Cr lying in the center.

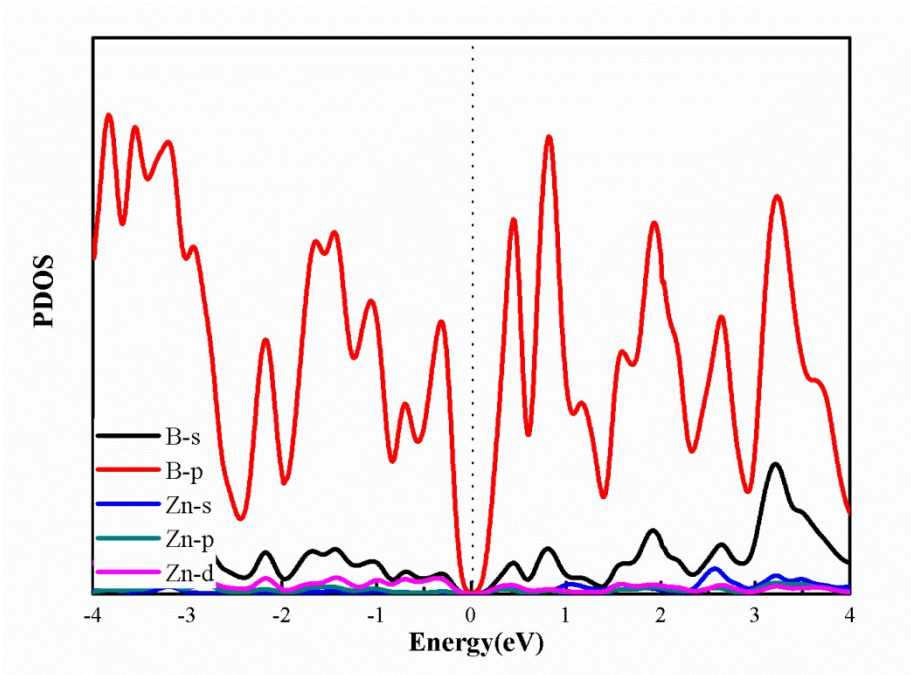


**Figure S4.** Projected density of states (PDOS) for 2D $Zn_2B_{40}$.