Electronic Supplementary Information (ESI) for Chemical Communication

Icosahedral B_{12}-Containing Core-Shell Structures of B_{80}

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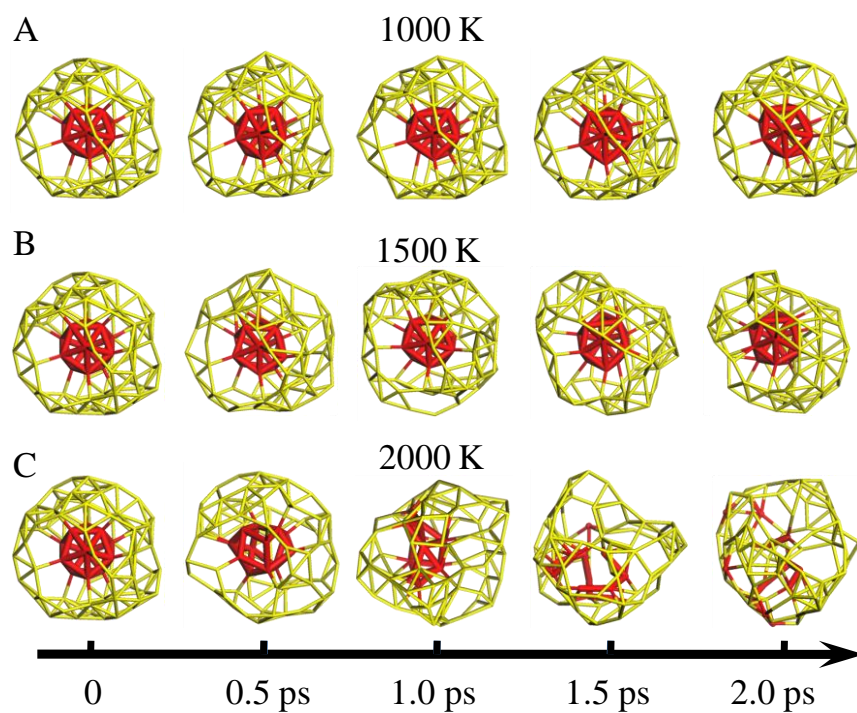E-mail: yuanlf@ustc.edu.cn

Figure SI-1. MD snapshots of I_h-B_{12} containing B_{80} in several time stages of MD simulation and at 1000 K, 1500 K and 2000 K, respectively.
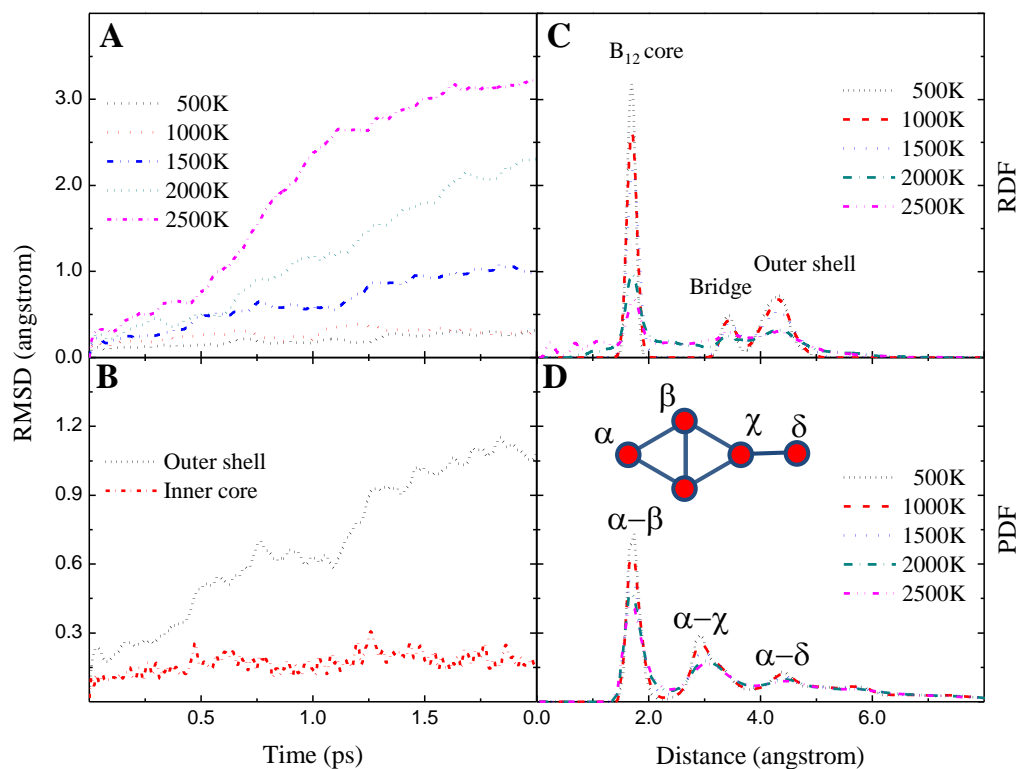
Figure SI-2. (A) Root mean squared distances (RMSDs) of I_h-B_{12} containing B_{80} at different temperatures. (B) RMSDs of outer shell and inner core at 1500 K. (C) Radial distribution functions (RDFs) and (D) B-B pair distribution functions (PDFs) at various temperatures. In computing RDFs, the centre of icosahedral B_{12} core is set as the origin of the coordinate
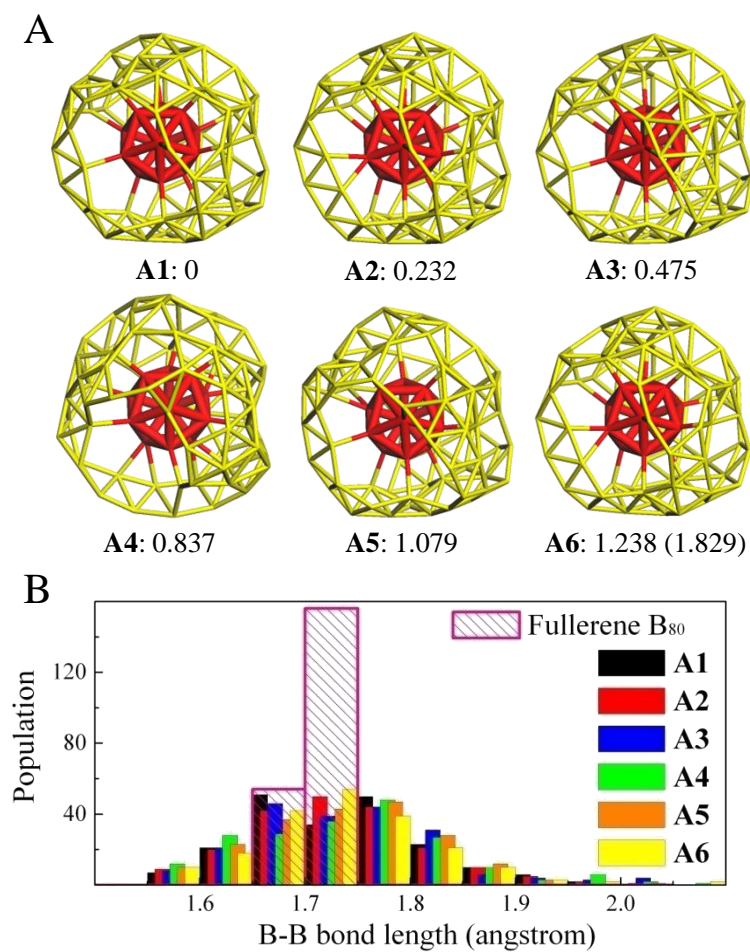
Figure SI-3. (A) Structures and relative energies (in eV), calculated at TPSS/6-311G(2d) //PBE/GTH-DZVP level, of the top 6 low-lying isomers **A1**-**A6**. Energy of the **A1** is set as zero, and the icosahedral B_{12} cores are highlighted in red. The relative energy between **A1** and **A6**, calculated by MP2/6-31G(d)//PBE/GTH-DZVP level, is given in parenthesis. (B) Distribution of B-B bond lengths of **A1**-**A6**, and that of the fullerene B_{80}.