Supporting information

Charge transport properties of tubular boron cluster based molecular junctions: A first-principles study

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1. Determination of the central boron cluster positions in molecular molecular junctions

In determining the position of the central cluster, the single-point energies of the molecular junctions were systematically scanned. Owing to the symmetry of the clusters, Fig. S1 exhibits a regular and periodic distribution of single-point energies. The difference between the maximum and minimum energies is found to be less than 0.35 eV. The most stable configuration was therefore selected as the final model for subsequent molecular junction optimization and charge-transport property calculations.
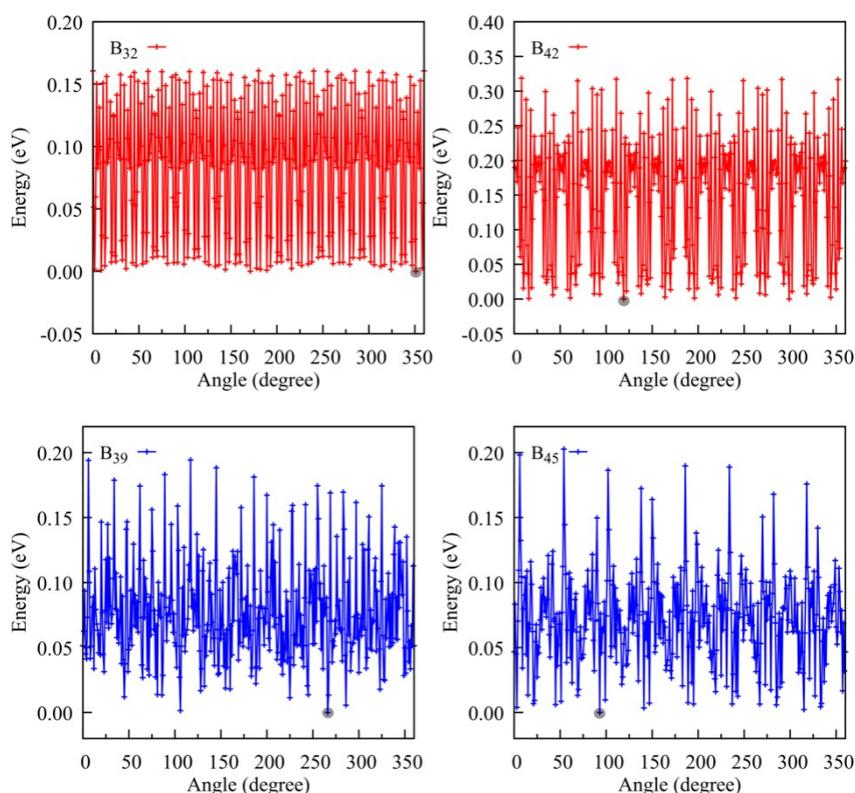

Fig. S1 Single point energy scanning diagrams of four molecular junctions.

2. K point grid testing based on B_{32} molecular junction

Figure S2 shows the k-point grid convergence tests for the B_{32} molecular junction. Test calculations were performed using a $3 \times 3 \times 1$ k-point grid. The resulting transmission functions were compared with those obtained using a $1 \times 1 \times 1$ grid. Very similar results were obtained for the two k-point samplings. This indicates that the smallest $1 \times 1 \times 1$ k-point grid is sufficient to capture the relevant transport characteristics of the
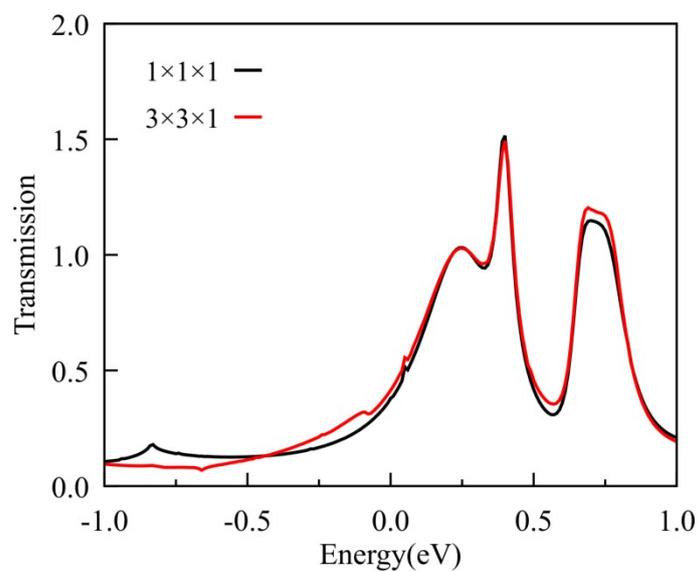
molecular junction.

Fig. S2 Zero bias transmission functions of the B_{32} molecular junction as simulated with the 1×1×1 k point grid (black) and 3×3×1 k point grid (red).

3. Real space distributions of the frontier molecular orbitals of the B clusters in free space

Figure S3 depicts the real space distributions of the frontier orbitals of the four boron clusters. The B_{39} and B_{45} clusters are open-shell systems, featuring distinct α-orbital and β-orbital distributions.
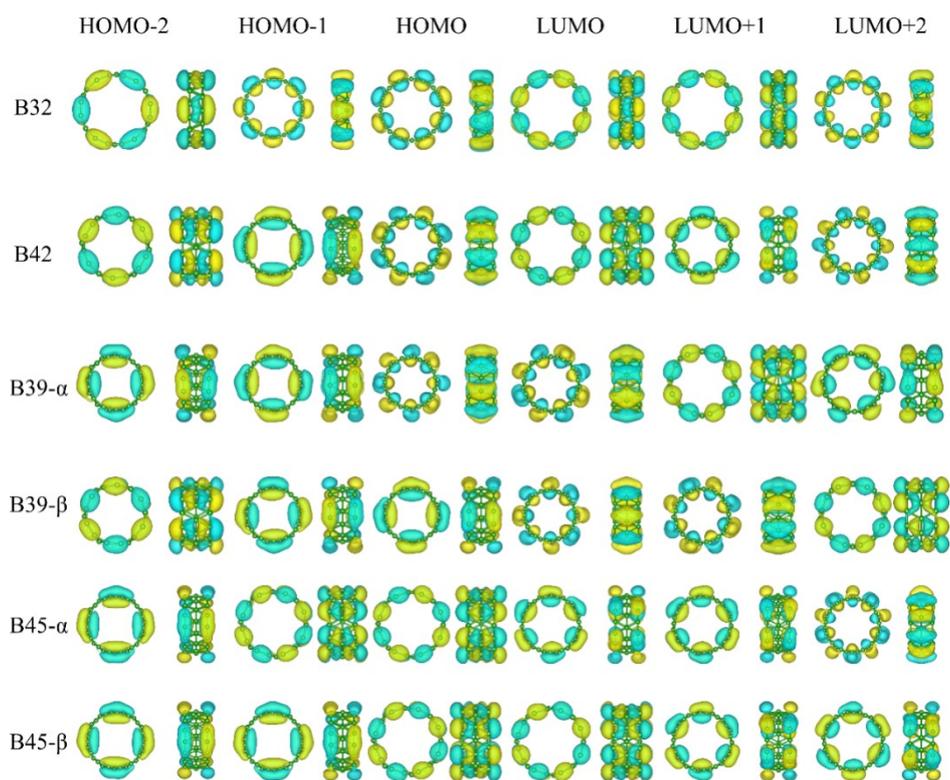
Fig. S3 The real space distributions of the frontier orbitals of the four boron clusters.

4. Transport properties of cage boron cluster B_{80}

Figure S4 depicts the structure of the constructed B_{80} junction and the calculated I-V currents. It can be seen that B_{80} presents nonlinear characteristics.
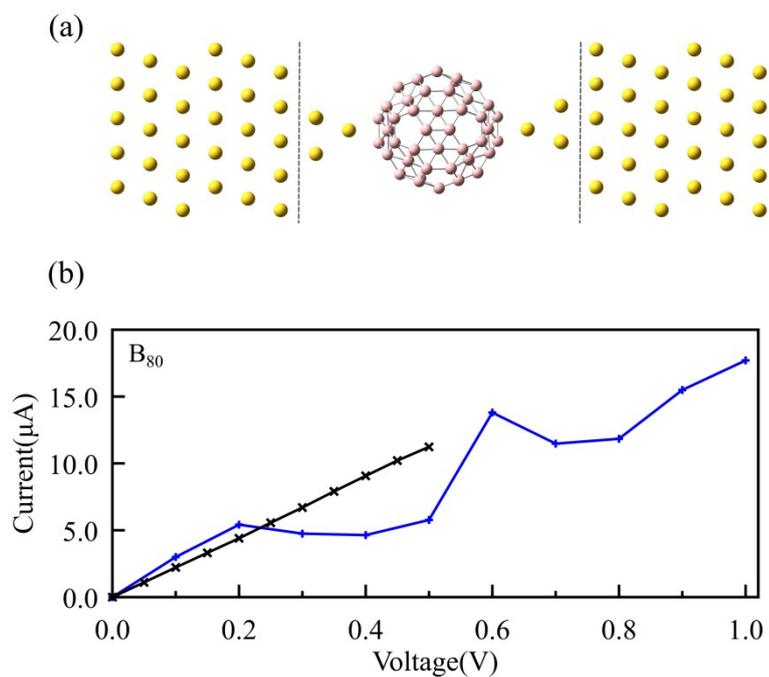
Fig. 4 (a) Configuration of the B_{80} junction. (b) Calculated I-V curve of the B_{80} junction(blue). For the sake of comparison, the I-V curve of the B_{80} junction (black) as reported by He et al. (J. Phys. Chem. C, 2010, 114, 4149) was also included in (b).