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Supplementary Information for

Electronic transport properties of the first all-boron fullerene B_{40} and its metallofullerene $Sr@B_{40}$

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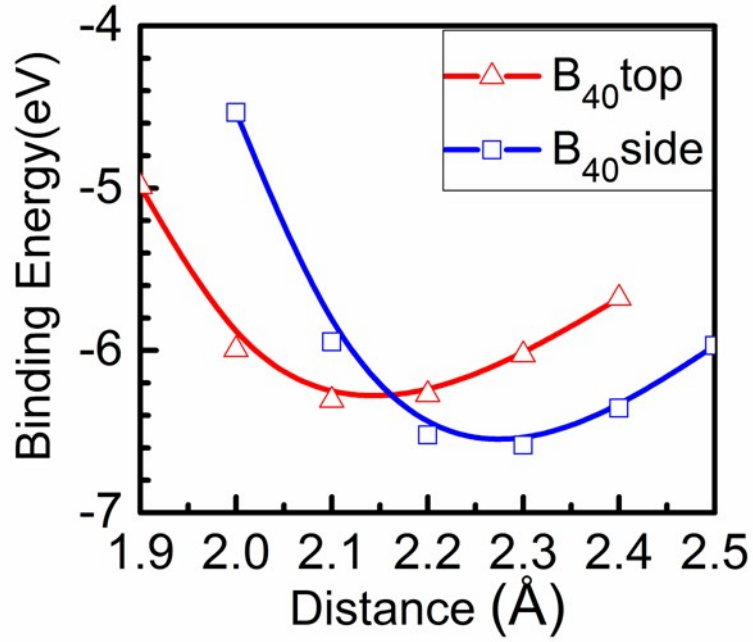

Fig. S1 Evolution of binding energies of the top- and side-contact for B_{40} with different contact distances.

The evolution of binding energies of the top- and side-contact for B_{40} with different contact distances are plotted Fig. S1. All the binding energies are negative, thus corresponding to a stable system. The evolutions of binding energy and total energy (shown in Fig. 2(b)) for B_{40} have the same trend, confirming the preferred contact structures.

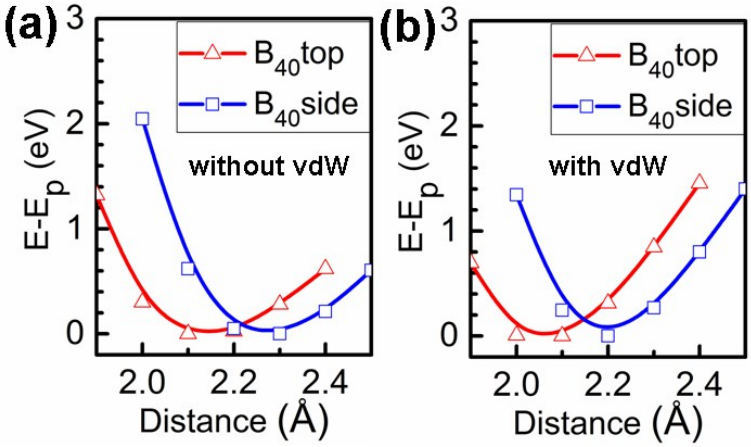

Fig. S2 Evolution of energies of B_{40} junctions with different contact distances, without (a) and with (b) van der Waals (VDW) interactions.

Fig. S2 gives the evolution of total free-energy of B_{40}top and B_{40}side junctions under the various contact distances, with and without considering the VDW interactions (based on the DFT-D3 method). There is no or little change of the preferred contact distance for B_{40} junctions when considering the VDW interactions. Namely, the preferred contact distance for B_{40}top junction is still 2.1 Å with or without considering the VDW interactions. That changes from 2.3 to 2.2 Å for B_{40}side junction when considering the VDW interactions, while giving rise to little change to the conclusions in the manuscript.