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Electron Transport in Boron Fullerenes

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Abstract- **The electron transport properties of B_{80} fullerene is studied using first-principles density functional theory in conjunction with the Landauer-Büttiker quantum transport formalism. The electron transmission in B_{80} fullerene is calculated to be much higher than that in C_{60} fullerene in the Fermi-level region. The enhanced transmission in the B_{80} fullerene is attributed to its spatially extended charge distribution in delocalized bonds.**

I. INTRODUCTION

The carbon fullerenes have shown a great potential in applications such as field effect transistors [1], spin valves [2], [3], electro-mechanic amplifiers [4], high temperature superconductors [5], to name just a few. By far the most common one is the buckminster fullerene, C_{60}, which has been shown to act as a semiconductor quantum dot [4]. Recently, boron related nanostructures have been the subject of several theoretical and experimental studies. Despite its preference to the three-dimensional (3D) structural motifs in natural structures, boron is shown to have planar or quasi-planar structures in small clusters [6], [7]. Theoretical studies have also shown the existence of two-dimensional (2D) boron sheets [8]-[10]. First principles calculations have predicted the most stable boron sheets and the corresponding single-walled nanotubes to be metallic [11], [12], in contrast to the diverse nature of single-walled carbon nanotubes ranging from metallic to semiconducting depending upon their chirality and diameter. The metallic nature of boron sheets and nanotubes is due to the unique bonding features of boron in forming multi-center bonds and having high coordination numbers [6], [7], [13]. Boron nanostructures are therefore expected to provide an alternative to carbon nanostructures for novel nanoscale devices.

Similar to carbon, boron fullerenes can be constructed from 2D boron sheet by following the isolated pentagon rule [14]. In addition, the hexagon rings prefer to have an extra boron atom at the center, following the Aufbau principle [6]. Just like in carbon, boron fullerene structures are predicted to be relatively more stable at certain "magic" numbers, such as B_{80} [15]. The goal of this paper is to explore the electronic and transport properties of boron fullerenes, namely B_{80}. The calculated results are compared with those of C_{60} fullerene to reveal differences, if any, between boron and carbon fullerenes.
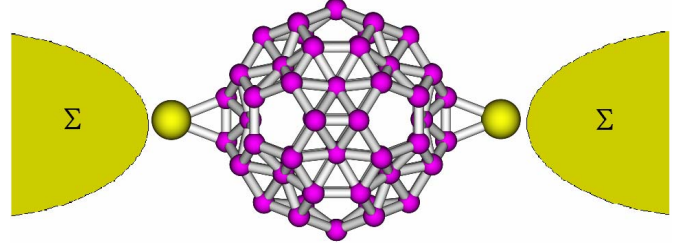
II. COMPUTATIONAL DETAILS

Fig. 1. Schematic illustration of the Au-B_{80}-Au molecular system considered for transport. The left/ right contact region is modeled by a Au atom and the rest of the semi-infinite electrode is a Au bulk reservoir, described by an effective self-energy term Σ.

The symmetry-constrained geometry optimization calculations were performed using Gaussian03 electronic structure program package [16] for B and C fullerenes considered using B3LYP functional form [17], [18] in the framework of density functional theory. The geometry of the two fullerenes were optimized with the use of STO-3G basis set. The choice of a relatively small basis set was made due to the computational requirements for large clusters. The bond lengths after relaxation are in good agreement with the previous theoretical study [15]. Finally single-point calculations at the optimized geometry were performed with a larger polarized basis set, 6-31G*. Table I lists the energies obtained using the 6-31G* set. The electronic transport calculations on the fullerenes coupled to semi-infinite Au electrodes (Fig. 1) were performed following the Landauer-Büttiker formalism [19]-[21]. The core scattering region was simulated by the extended molecular complex, Au-fullerene-Au where atomic scale contacts were used for the fullerene molecule. The LanL2DZ basis sets for boron and gold atoms were used for transport calculations.

The total current in the Au-fullerene-Au device can be obtained by the following equation

$$I = \frac{2e}{h} \int_{-\infty}^{\infty} dE\, T(E,V)[f(E-\mu_1) - f(E-\mu_2)]$$

where, μ_1 and μ_2 are the electrochemical potentials in the two contacts under an external bias V, $f(E)$ is the Fermi-Dirac distribution function. $T(E,V)$ is the electron transmission function which can be calculated from a knowledge of the molecular energy levels and their coupling to the metallic contacts. Additional details of the calculations can be found elsewhere [3], [22].

In the scattering region, the point contacts of the gold leads were represented by a single atom [3], [23], and the bulk effect was implicitly included by the self-energy term Σ. The bridge site between two six-membered rings of the fullerene was taken to be the binding site of the metallic contact atom [3]

with the bond distances of 2.2 Å and 2.4 Å, Au-B and Au-C were kept at, respectively.

III. RESULTS AND DISCUSSION

A. Electronic Structure

The optimized structure of B_{80} fullerene is shown in Fig. 1 together with the contact Au atoms. Symmetries, binding energies E_b, and the frontier orbital gaps, obtained as the energy difference between the highest occupied (HO) and the lowest unoccupied (LU) molecular orbitals (MOs) of the fullerene molecules C_{60} and B_{80} are listed in Table I. The B_{80} molecule can be viewed as a derivative of C_{60}-like structure by adding extra atoms at the center of all hexagons [15]. It consists of 12 pentagons and 20 centered-hexagons holding I_h symmetry. The centered-hexagons are cross-linked through the global molecule. The bond lengths after relaxation are in good agreement with the previous theoretical study (using PBE/plane-wave basis sets, ultrasoft pseudopotentials) [15].

TABLE I
Symmetries, binding energy (E_b) and the HOMO-LUMO gaps of the isolated fullerene molecules at B3LYP/6-31G* level.

fullerene	Symmetry	E_b (eV/atom)	HOMO-LUMO Gap (eV)
B_{80}	I_h	5.17	2.12
C_{60}	I_h	6.97	2.74

B. ElectronTransport

The calculated transmission functions and currents of B_{80} along with that of C_{60} are shown in Fig. 2 and Fig. 3 respectively. The transmission function, in general, reflects the intrinsic transmission characteristics of the fullerene molecule. The large HOMO-LUMO gap of the isolated C_{60} molecule reflects itself in a vanishing transmission gap in the near-Fermi region [23]. The closest transmission peaks at ~0.7 eV (labeled by * in Fig. 2) are due to LUMO-derived states, i.e. two pure C_{60}-LUMO states and one hybrid state of C_{60}- LUMO and Au (note that the isolated C_{60} has 3-fold degenerate LUMOs). These results are consistent with an earlier theoretical study using the non-equilibrium Green's function (NEGF) method [24], except the shift in peak position about 0.6 eV towards higher energy. It should also be pointed out that the previous study [24] utilized Au(100) surface to model the metal electrode. A higher charge transfer of 0.7 e from Au to C_{60} was predicted there as compared to the current value of 0.22 e, which indicates a higher population of C_{60} LUMO states.

The B_{80} fullerene system has a non-negligible transmission at the zero injection energy, which arises from the diffusive transmission peaks due to the Au-molecule hybrid states in the near-Fermi region. The gap in the transmission due to the HOMO-LUMO gap is still tractable for B_{80}. Within the gap, there are two metal induced gap states (MIGS) for the B_{80} extended molecule. They arise from the hybridization of Au 6s and B_{80} states located mainly on the B-B bridge sites biding to Au contacts, which, however, do not show any close affinity to any of the isolated B_{80} molecular states near the pseudo Fermi level E_F. The HOMO state is shown to be rather delocalized, leading to a very diffusive transmission without showing a distinguishable peak. The LUMO state of the system, which is

more localized at the two Au-bonding region, accounts for the sharper transmission peak shown at ~0.2 eV (labeled by ^ in Fig. 2) for B_{80}. The charge transfer from Au to B_{80} is about the same as to C_{60}.
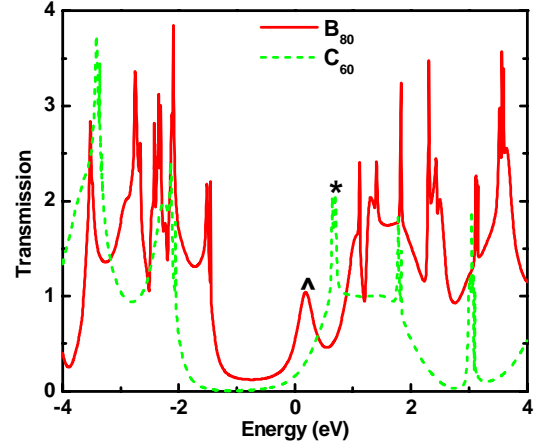

Fig. 2. Transmission functions for B_{80} and C_{60} molecular systems. Zero of the energy is aligned to the pseudo Fermi level. Several transmission peaks are labeled for discussion in the text.
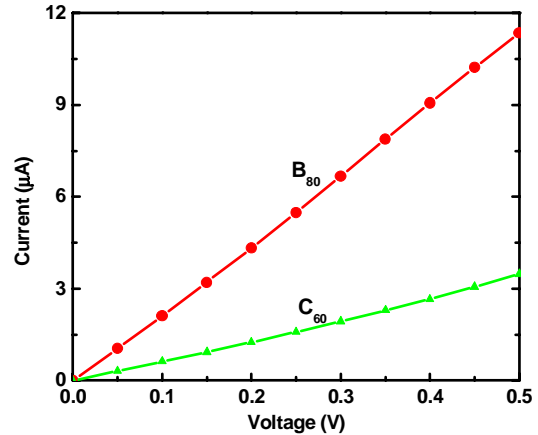

Fig. 3. Current-voltage curves for B_{80} and C_{60} molecular systems.

IV. SUMMARY

In summary, the boron family of engineered nanomaterials has appeared to have unique chemical bonding and electronic properties. In this work, we have studied the electron transport properties of one of the most stable boron fullerenes, B_{80}. The calculated results reveal a substantially enhanced transmission as well as tunneling current for B_{80} as compared to C_{60}. In the case of the former, a non-vanishing transmission near E_F is observed, while in the latter case a large gap in transmission near E_F is observed, resulting from its semiconducting property.

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