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Probation of charge transport with chalcogens as linker group for C_{20} fullerene

Milanpreet Kaur, Ravinder Singh Sawhney, Derick Engles*

Department of Electronics Technology, Guru Nanak Dev University, Amritsar, Punjab, India

Abstract

In this paper, we explored the superconductive nature of fullerenes for its applications in molecular electronics. The fullerenes that we exploited for this research work were C20 and its three variants; formed by anchoring with oxygen, sulphur and selenium atoms from chalcogens group (Group xvi) of periodic table. Next, the self-consistent calculations using Extended Hückel Theory (EHT)–Non Equilibrium Green Function (NEGF) were performed in extended molecule configuration in which fullerene molecule was bridged in gold electrodes. The quantum characteristics of these variants were scrutinized and compared, which demonstrated the electrical superiority of pure C20 molecule over the rest of its variants.

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*Keywords:*Non Equilibrium Green's Function (NEGF); Extended Hückel Theory (EHT); Molecular electronics; Chalcogens (Group xvi)

1. Introduction

In 1985, H. W. Kroto, R. F. Curl and R. E. Smalley discovered the new molecular allotrope of carbon, fullerenes [1] and were awarded the Nobel Prize in chemistry in 1996 for this groundbreaking scientific finding. However, it was in 1990 when C60 was first available in multigram amounts with the preparation procedure of Krätschmer and Huffman [2]. This upshot expanded its horizon [3-5] and led to modification of the chemical structure of C60

* Corresponding author.
*E-mail address:*mkb1313@yahoo.com

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forming various fullerene derivatives [6]. The iconic shape of fullerenes—hollow polyhedral built of sp2-hybridized carbon atoms— with outstanding structural [7, 8], magnetic [9-11], superconducting [12-15], electrochemical [16-17] and photophysical properties [18, 19] is strongly associated with the field of molecular nanotechnology. The discovery of superconducting phenomenon in alkali-doped C60 [12, 20] and in C70 [13] has attracted much notice as examples of a new class of superconductors. In this context, the smaller fullerenes are the most interesting as they maintain the curvature properties without compromising stability [21- 24]. The synthesis of the smallest fullerene, C20, was started from the stable C20H20 molecules by H. Prinzbach et.al. [25]. More work on this front has been proposed by Spagnolatti et.al. [26]. The first-principles study of structure and quantum transport properties of C20 fullerene molecule was proposed by An et.al. [27]. In this paper, we studied pure C20 and its variants; formed by anchoring with three of the chalcogens atoms i.e. oxygen, sulphur and selenium in two probe configuration.

2. Modelingand simulation

We modeled the smallest possible fullerene molecule, C20 which is the polyhedral carbon cage with 12 pentagonal and zero (n/2-10) hexagonal faces. The electronic configuration of the constituent carbon atom is 1s2 2s22p2. It is assumed that in a fullerene molecule, two 1s electrons of each atom belong to core with other two 2s electrons forming molecular bonds and rest two 2p electrons are delocalized. Hence, in C20 molecule, there are 40 delocalized electrons which would be responsible for the electrostatic energy inside-outside the spherical cage of molecule.

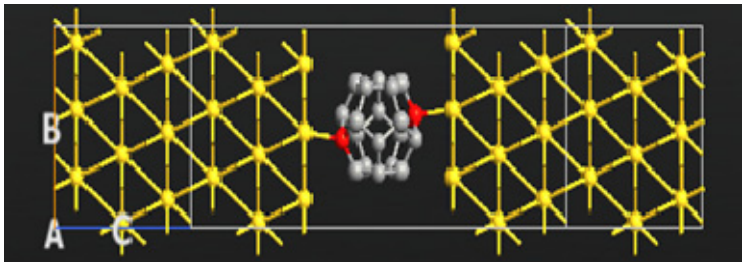

Fig. 1.Gold electrodes stringed C20 molecule forming an “extended molecule”. Red coloured atoms indicate the position of anchored atoms that were replaced by oxygen, sulphur and selenium.

The pure C_{20} was placed in-between semi-infinite-gold electrodes forming the single molecular device (fig. 1). In single molecular device, system is divided into 3 parts: (1) left electrode, (2) central scattering region and (3) right electrode. A central scattering region consists of some layers of electrodes and a molecule under observation. Similarly, for the variants of fullerene molecule, the two probe configurations were formed by replacing the anchor atoms of molecule by oxygen, sulphur and selenium atoms respectively. The chalcogen anchor elements are two electrons short in octet and show the increasing metallic character as the atomic number increases within the group. This nano-setup is said to be placed in the isolated environment, where the interactions with the external environment are neglected to observe the quantum effect of charge transport in the single molecular device at 1-D level for the superconductive characteristics.

The simulation and calculations were done in Virtual Nano Lab (VNL), the graphical interface of the Atomistic Tool Kit (ATK) provided by Quantum Wise [27]. Although there are number of the calculation methods available for the molecular electronics but we preferred to use the semi empirical approach of Extended Hückel Theory (EHT) because of its faster response and higher accuracy rates for mono particle calculations. Also, the Hamiltonian matrix elements could be defined by very few parameters in the Extended Hückel model. Next, for the self-consistent calculations, the density matrix was calculated from the Hamiltonian using Non-Equilibrium Green's Function (NEGF) for device systems [28]. Once the self-consistent non-equilibrium density matrix was obtained, it was possible to calculate two electrical characteristics of the system- current and conductance.