Journal of Physical and Theoretical Chemistry
of Islamic Azad University of Iran, 13 (1) 9-16: Spring 2016
(J. Phys. Theor. Chem. IAU Iran)
ISSN 1735-2126

Electronic transport in Si and Au monoatomic chains considering strongly correlation effect, a first principle study

Mansoureh Pashangpour[*1] and Vahid Ghaffari [2]

[1] Department of Physics, Islamshahr Branch, Islamic Azad University, Islamshahr, Iran
[2]Central Tehran Branch, Islamic Azad University, Tehran, Iran

Received February 2016; Accepted April 2016

ABSTRACT

We have investigated structure and electronic properties of Au and Si liner chains using the first-principles plane wave pseudopotential method. The transport properties and conductance of these two liner chains are studied using Landauer approaches based on density functional theory (DFT). We obtain density of states and band gap using Kohn-Sham and Wannier functions as well as quantum conductivity and current for Au and Si liner chains. We study the effect of Hubbard U on quantum conductivity and current for Au liner chain within DFT+U for strongly correlated systems. We compare the source of the states around Fermi level of these systems that have important role in conductivity. We present I-V characteristics of the Si and Au liner chain. Results show Ohmic behavior of current flow in the liner chains in terms of applied bias voltage. We show that Hubbard U correction removes the unphysical contribution of d electrons to the conductance of Au liner chain, resulting in a single transmission channel and a more realistic conductance of $1G_0$that is in good agreement with experimental results. Our calculations reveal that monatomic chains of Si and Au are metallic therefore they can be used as connectors between nanoelectronic devices.

Keywords: Density functional theory; Density of state; Quantum transport; Strongly correlated system; Wannier function

INTRODUCTION

Nanoelectronic, electronics at the nanoscale, represents the next years' technological challenge since low dimensional forms of materials have properties quite different from those of their bulk structures. One-dimensional systems such as nanowires are believed to be the most important building blocks for the next generation of electronic devices. In particular, metallic nanowires are attractive because of their unique electrical properties. Metallic nanowire's relevances in nanotechnology are their usage as interconnecting between nanodevices, fabrication of nanoscale field-effect transistors and circuit application[1-3].Semiconducting and insulating nanowires are also of importance in the context of design and operation of integrated nanoscale devices.

In the last years, a combination of *ab initio* density functional theory (DFT) calculations together with the description of transport properties in a Landauer framework[4] has demonstrated its ability to describe small bias coherent transport in nanojunctions[5-9].

[*]Corresponding author: poor@iiau.ac.ir

The organization of this paper is as follows: In Section 2 the computational method is discussed. In Section 3 we investigate the electronic structure of infinite monoatomic chains of Au and Si atoms, using density functional theory within the generalized gradient approximation (DFT-GGA) calculation based on plane waves and norm-conserving pseudopotentials using periodic boundary conditions.Also, we considerHubbard U for a GGA+U calculation ofAu monoatomic chain. Finally, in Section 4 the electrical conductance of these systems are studied. The electronic and transport properties of these structures are analyzed using first-principles methods. From the DFT and DFT+U KS eigenfunctions, we obtain an orthonormal set of maximally localized Wannier functions [10], which are used as a basis set in the calculation of quantum transport. Calculations of the quantum conductance have been obtained using the WanT package [11] that is performed using the Fisher-Lee formula [12].We apply this scheme to realistic systems, Au and Si monoatomic chains [13]and we study the effects induced on transport properties by the wannier functions via GGA and GGA+U approximation.

METHOD

The first-principles calculations are performed within the framework of DFT and the *ab initio* pseudopotential plane-wave method using the PWSCFcode of the Quantum ESPRESSO distribution [14]. The calculations are performed with GGA where the Perdew-Burke-Ernzerhof (PBE) (non NLCC) pseudopotential [15] was employed. For the pseudopotential generation Brillouin Zone integration was performed using 8×1×1 Monkhorst and Pack special point grids [16] with a smearing width of 0.01 Ry using Gaussian smearing technique in order to smooth the Fermi distribution. A plane wave basis set is used to expand the Kohn-Sham orbitals. The energy cut-off for the wave function and the charge density are 40 Ry and 400 Ry, respectively.

Calculations of the quantum conductance have been obtained using the WanT package [11] that is performed using the Fisher-Lee formula [12]. This code provides an integrated approach for the study of coherent electronic transport in low-dimensional and extended nanostructures. The core methodology combines DFT, plane-wavesand pseudopotential calculations with a Green's functions method based on the Landauer formalism[4] to describe quantum conductance. Zero-temperature conductance through a region of non-interacting electrons is related to the scattering properties of the region itself via the Landauer formula in this code.

ATOMIC AND ELECTRONIC STRUCTURE CALCULATIONS

The 1D structure of Au and Si chains are treated within supercell geometries as orthorhombic cell with four atoms (Fig. 1).All the atomic positions and lattice parameters of the structures have been optimized by minimizing forces on atoms and the stress on the structures.

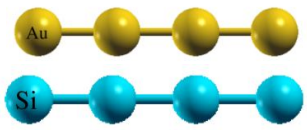

Fig. 1.unit cell of Au and Si liner chains.

The equilibrium lattice constant of the Si linear chain (Si-LC) and Au linear chain (Au-LC) are obtained as 2.16 Å and 2.49 Å using plane wave and formation energies are calculated 4.28 eV and 2.2 eV, respectively. The Kohn-Sham electronic band structure from the PW calculation is

shown for the relaxed geometry in Fig. 2 and Fig. 3. From the DFT KS eigenfunctions, we obtain an orthonormal set of maximally localized Wannier functions (MLWF's) [10], which are used as a basis set in the calculation of quantum transport. MLWF's allow to bridge plane-wave electronic structure and lattice Green's function calculations in a coherent fashion. DFT-GGA levels from the PW calculation are represented in Fig. 2 and Fig. 3. We verified that the diagonalization on the MLWF basis closely reproduces the PW results.

The character of the strong binding for Si-LC is given by the formation of double bonds between adjacent atoms; one of them, the σ bond, is composed of *s*- and p_x-valence orbitals. The second bond is the π bond made by p_z and p_y atomic orbitals perpendicular to the chain axis (x direction),while the binding for Au-LC is formed with *s*- and five *d*-orbitals. The *d*-orbitals of Au-LC are located below of E_F. We obtain that the top of the 5d xz and xy bands of Au are slightly above E_f (Fig. 4),while transport experiments in Au chains indicate that these bands do not cross the Fermi level [18].Considering strongly correlation effect for Au atoms in Au-LC within DFT+U calculation cause a shift of *d*-orbitals to lower levels.

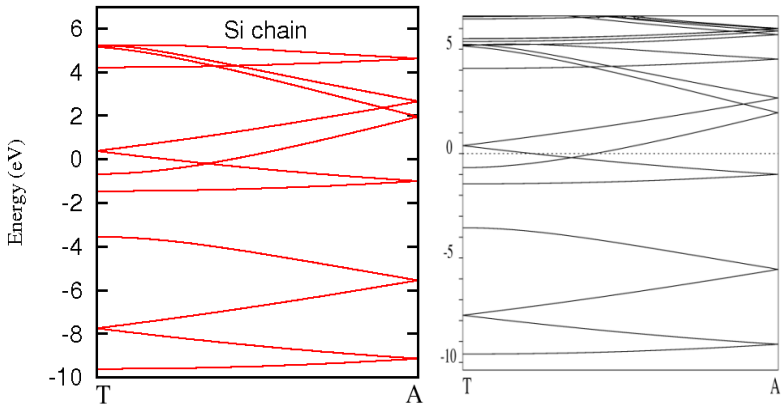

Fig. 2. Electronic band structure of Si-LCis obtained from MLWF (left) and DFT-GGA calculations with KS states (right). The Fermi level is set to zero.

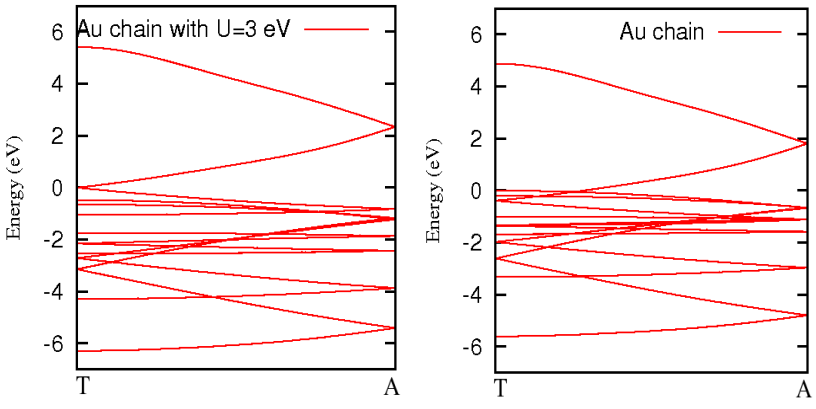

Fig. 3. Electronic band structure of Au-LC is obtained from DFT (right) and DFT +U (left) calculations with MLWF. The Fermi level is set to zero.

There is a small charge transfer, 0.14 e, from *s*-state and *p*-states to *d*-states of Au within GGA+U calculation of Au-LC. Projected density of states (PDOS) of Au atoms in Au-LC with GGA+U calculations how upward shifts for *s*-state and *p*-states while down shifts are obtained for *d*-states respect to GGA calculation of Au-LC (Fig. 4).

A simulated STM image of the Au-LC chain is obtained in (110) and (101) surfaces, the chain axis is x direction. The image is obtained by integrating the density of states from the bias potential to the fermi energy [17].

CALCULATION OFELECTRICAL CONDUCTIVITY

By Landauer approach we have investigated the electrical transmission of 1D dimensional Au-LC and Si-LC. The wannier functions (WFs)' centers for Si-LC are made by hybridization of *s*-, p_x, p_y and p_z atomic orbitals and for Au-LC are formed with *s*- and five *d*-orbitals. In Fig. 6 we show the conductance of the gold and silicon chains for the relaxed geometry are obtained using the Landauer formula, the DFT and DFT+U KS electronic structure. WF's are considered as one *s*- and five *d*-orbitals on each Au atoms for Au-LC. The conductance of Au-LC at the Fermi level appears to be 1 (in units of $2e^2/h$)within DFT calculation and it has *s*-like character that is in good agreement with others work [19].The Fermi level is at the limit of the onset of the *d*-like states. Considering DFT+U framework, interesting results are obtained in Au-LC transport properties, the *d*-levels of Au atoms shift to lower levels and around Fermi level just *s* state of Au atoms appears. The DFT prediction of the conductance reaches $6e^2/h$ below the Fermi level for the pristine Au-LC in the spin-unpolarized case while one would expect a value around $G_0=2e^2/h$ from a single spin-

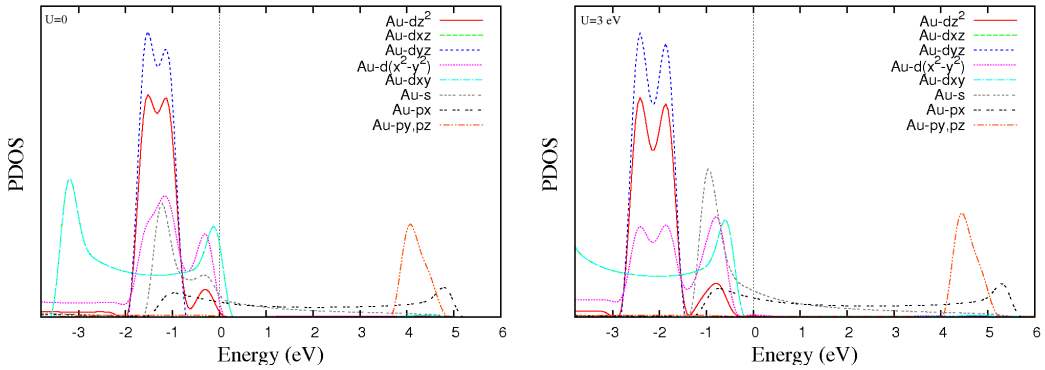

Fig. 4. Projected density of states of Au-LC is obtained from DFT (left) and DFT +U (right) calculations with KS states. The Fermi levelis set to zero.

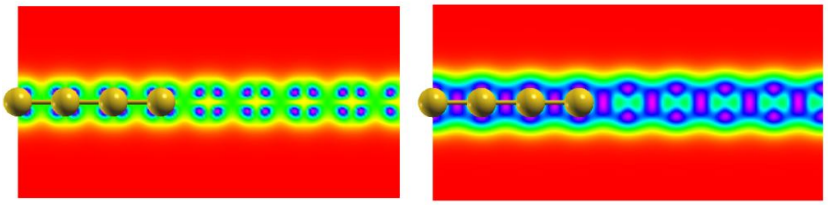

Fig. 5. A simulated STM image of Au-LC is obtained from DFT (left) and DFT +U (right).

degenerate channel, as shown by experiments on clean Au nanocontacts [20] that it is obtained within our DFT+U calculation. Decreasing the number of states of Au-LC around E_F reduces considerably the conduction and I-V character.

WF's are considered as *s*-, p_z, p_y atomic orbitals on each Si atoms and p_x atomic orbital on midpoint of Si bonds for Si-LC. Around the Fermi level, The Si-LC has a doubly degenerate π band and a σ* band crossing the Fermi level leading to 3(in units of $2e^2/h$). The conductance first reaches to 2below Fermi level with two σ bonding bands and then increases to 4 in up of Fermi level with both a degenerated π band and a dipped σ* band. Around Fermi level, Si-LC conductance is considerable in comparison to Au-LC conductance.

The states around Fermi level play important role in conductivity. DOS at the top of Au-LC Fermi level decreases suddenly but the states around Si-LC Fermi level are considerable that they affect the chain's conductivity (Fig. 7 and Fig. 8). From the analysis of the eigen channels contributing to the total conductance of Au-LC, we have found one open channel mainly formed by the *s* orbital.

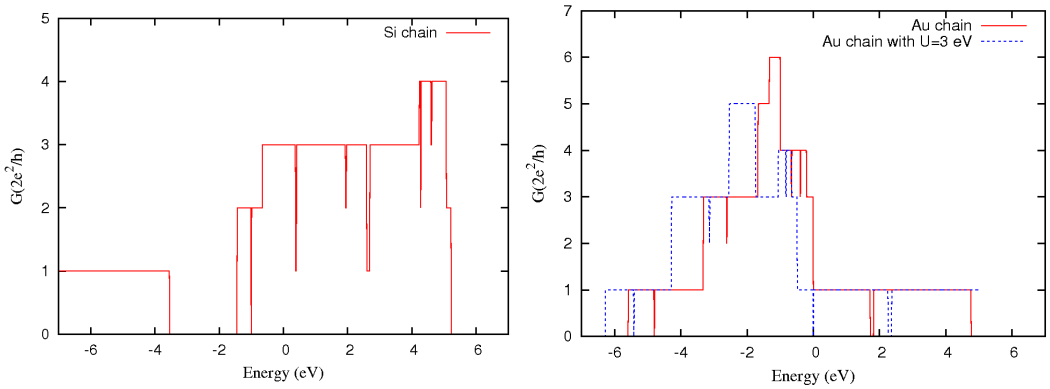

Fig. 6. Calculated quantum conductance of Si and Au liner chains in terms of bias voltage. Fermi level is set to zero.

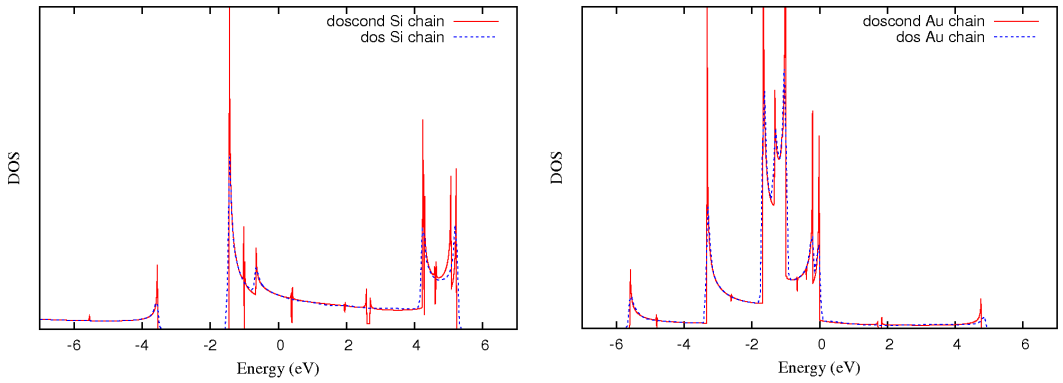

Fig. 7.DOS and DOScond of Au and Si liner chains. Fermi level is set to zero.

In Fig. 9 the I-V curves of the two cases have been depicted. The Fermi level of the left electrode shifts upward with respect to that of the right electrode when the bias voltage is applied. Therefore, the current starts to flow only after the valance band maximum of the left electrode reaches the conduction band minimum of the right electrode. The I-V curve of Si-LC has better Ohmic behavior than Au-LC. Hubbard U introduces significant changes in I-V curve of Au-LC and its Ohmic behavior is limited to interval -1 to +1 V for bias voltage. Slop of I-V curve defines conductivity of LCs that is similar for Au-LC and Si-LC with DFT calculation. The conductivity of Au-LC is reduced with DFT+U calculation (Fig. 9 (left)).Calculating the slopes of these curves, we obtain the conductance of Au-LC with and without Hubbard U and Si-LC to be 1.414, 0.772 and 2.14 (μA/V), respectively.

Minimum current at zero bias voltage is 5.74×10^{-9}µA and 8.1×10^{-11}µA for Au-LC within DFT and DFT+U calculations that limits the usage of Au-LC for digital switching, where high on/off ratios are necessary, while the minimum current of Si-LC is zero.

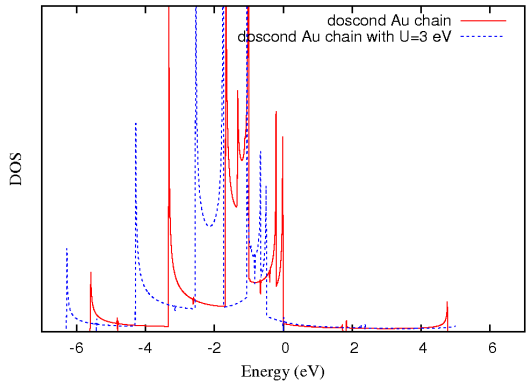

Fig. 8.DOS of Au liner chain within DFT and DFT+U calculations. Fermi level is set to zero.

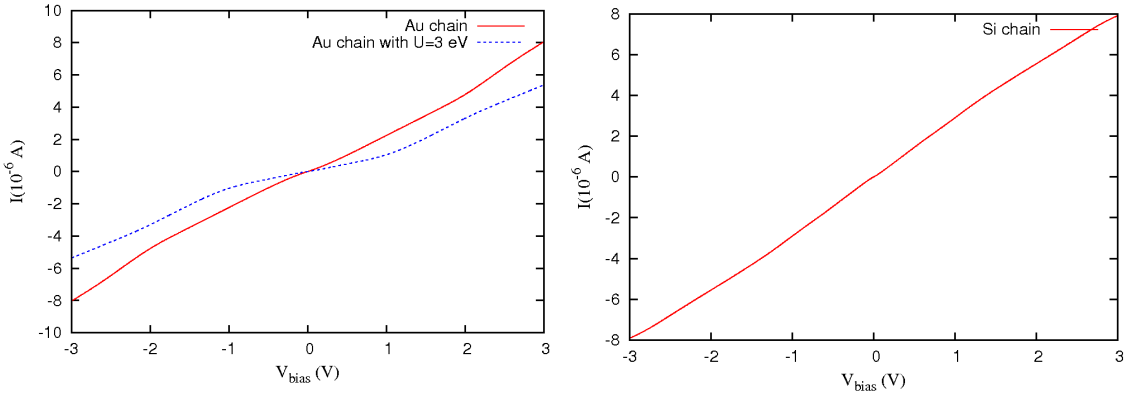

Fig. 9.I-V curve of Au and Si liner chains in terms of bias voltage. Fermi level is set to zero.

CONCLUSION

In conclusion, using first-principle calculations we have systematically studied the structure, electronic and transport properties of Si and Au nanochains. The calculations are done utilizing the density functional theory through the pseudopotentials and plane-waves method within the generalized gradient approximation and also with Hubbard U.Hubbard U introduces significant changes in I-V curve and conductivity of Au-LC. The Ohmic behavior is limited to interval -1 to +1 V for bias voltage. Slop of I-V curve defines conductance of LCs that is similar for Au-LC and Si-LC with DFT calculation. DFT+U calculation affects the Au-LC conductivity. We have calculated the conductance of a these systems by taking into account Landauer formalism. Results show that Si-LC conductance is considerable in comparison Au-LC conductance around Fermi level since the states decreases suddenly at the top of Au-LC Fermi level respect to states of Si-LC. Both two liner chain have metallic behaver because of their zero energy gap. Also, results show the I-V curve of Si-LC has better Ohmic behavior than Au-LC.

ACKNOWLEDGMENT

The authors gratefully acknowledge the financial and other support of this research, provided by the Islamic Azad University, Islamshahr Branch, Tehran, Iran.

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