International Journal of Research in Engineering and Science (IJRES)
ISSN (Online): 2320-9364, ISSN (Print): 2320-9356
www.ijres.org Volume 10 Issue 9 ǁ September 2022 ǁ PP. 315-319

Structural and Electronic properties of Al and Pt wires: A DFT study

Kumar Saurabh Yadav[1], B.S. Bhadoria[1*], Jitendra Kumar[2*]
[1]*Department of Physics, Bundelkhand University, Jhansi, U.P. India*
[2]*Department of basic sciences, Babasaheb Bhimrao Ambedkar University, Lucknow, U.P. India*
Corresponding Email:- bsbhadoria@yahoo.com,vinjitu@gmail.com

ABSTRACT
In this article, we present electronic structure, Fermi energy, total energy, transmission coefficient, band structure and density of states for atomic wires of Al and Pt. The electronic structure analysis is based on a first-principles density functional method. We also compare our result with available previous theoretical data and it can be clearly seen that this current results of the work are in good agreement with the reported results.
KEYWORDS*- density functional theory (DFT), density of states (DOS), band structure*

Date of Submission: 02-09-2022 Date of acceptance: 15-09-2022

I. INTRODUCTION

Electronic materials in bulk and thin film structures, where charge carriers move freely in three-dimensional space, have attracted many investigations due to their unique magnetic, electronic and optical properties. Furthermore, nanostructured systems such as quantum dots, nanocolumns and nanowires have attracted many studies because of their specific functionality [1-6]. For example, nanodots arrays have shown some potential applications such as effective enhancement of the electric field of incident light, controlling photon emission by multiple excitations, tuning the on/off ratio on nano spin-diodes, and non-volatile memory devices [7-15]. In addition, nanowire systems are also of great interest for future device applications, such as optoelectronics and magnetic memory devices, due to their unique properties [16-22].

Proton exchange fuel cells are highly efficient in converting hydrogen and oxygen into water and electrical energy. Significant advances have been made in fuel cell technology, and although many kinds of novel catalysts have been developed in recent years, platinum is still the most promising and commonly used catalyst, due to its high stability in the aggressive chemical environment of strongly oxidizing and highly acidic conditions, high electrochemical potentials and gradients, and reactive chemical intermediates in proton exchange fuel cells. Platinum (Pt)- based nanowires can give excellent performance as electrochemical catalysts in low temperature proton exchange fuel cells. Several preparation methods have been developed for this kind of application. Platinum based nanowires can give excellent performance as electrochemical catalysts in low-temperature proton exchange fuel cells. Several preparation methods have been developed for this kind of application [23-27].

In this article, we present electronic structure, Fermi energy, total energy, transmission coefficient, band structure and density of states for atomic wires of Al and Pt. The electronic structure analysis is based on a first-principles density functional method.

II. COMPUTATIONAL METHODOLOGY

All calculations were performed using the Born–Oppenheimer approximation within the framework of density functional theory and employing the plane-wave basis set and pseudo potentials employed in the Quantum Espresso package implemented at Compute Canada. Self- consistency calculations following the Kohn–Sham formalism were used to solve single particle equations with Quantum Espresso. For all DFT calculations we used the local density approximation in its Ceperley and Alder form, as estimated by Perdew–Zunger for the exchange–correlation functional. To better approximate the relativistic effects, the radial Dirac equations derived from the scalar relativistic approximation were used. The configuration of $3s^2$ $3p^1$ for Al atoms was treated as the relevant valency using the generated USPP pseudo potentials for LDA based functionalities implemented in Quantum Espresso [28-31].

III. RESULTS AND DISCUSSION

Now we will study the structural and electronic properties of Al and Pt wires. The geometries of Al and Pt wires has been optimized by using quantum espresso software (open source) which areshown in figure 1. The lattice parameters for Al wire are 16.1557Å, 4.03893Å and 4.03893Å hasbeen used for this calculation and for Pt wire are 11.9303Å, 3.97677Å and 3.97677Å. The total energies for Al and Pt wires are -64.84476189 Ry and -1066.0574 Ry. The Fermi energies for Aland Pt wires are is 8.2690 eV and 16.78eV has been calculated. The relation between transmission coefficient and energy has been shown in figure 2 and 3.

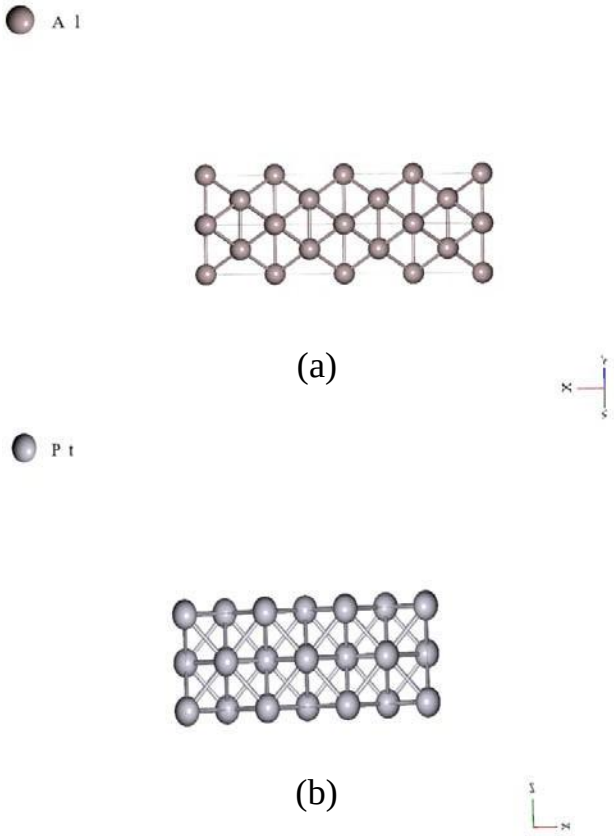


Fig.1:- Al and Pt wire with orthorhombic unit cells

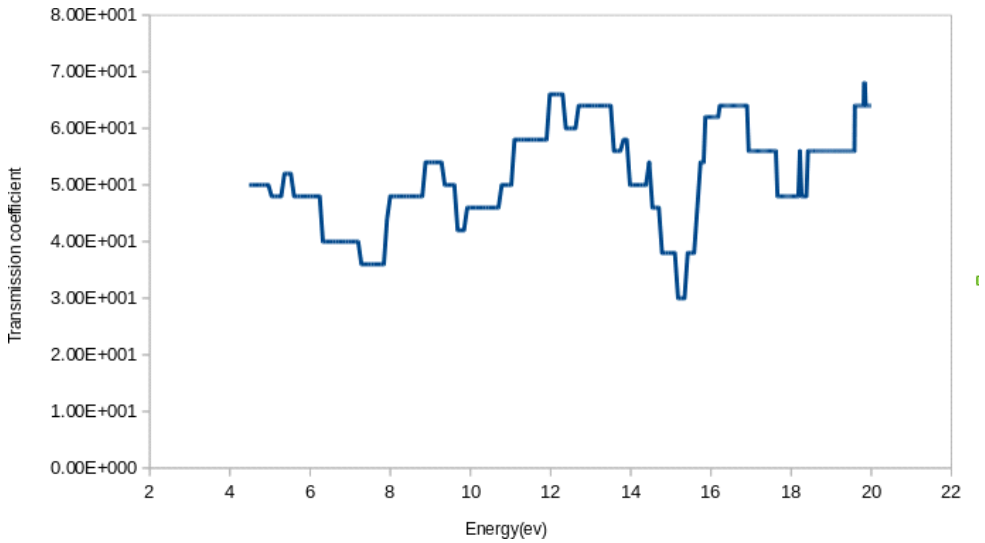


Fig.2:- Transmission coefficient of Al wire

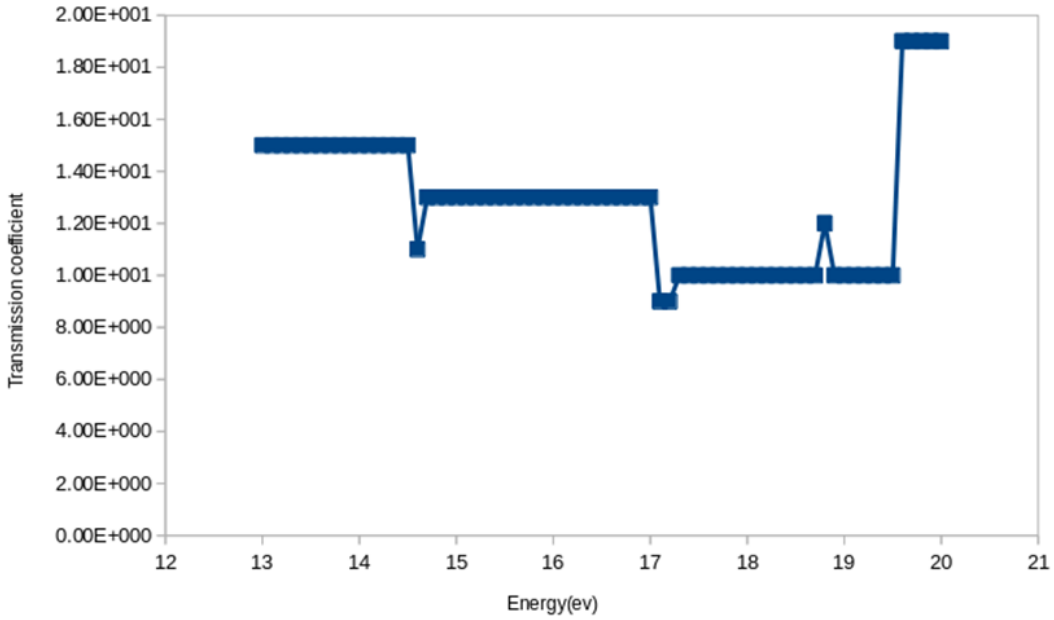


Fig.3:- Transmission coefficient of Pt wire

The density of states (DOS) plays an important role in determining the transition rates; The DOS is not immutable, in other words it is not a quantity that is fixed by nature, but the DOS can be manipulated to improve device theory. The DOS of a classical system is the number of states of that system per unit energy, expressed as a function of energy performance. The DOS is also central concept in the development and application of RRKM. The DOS of Al and Pt wires are shown in the Figure 4 and 5.

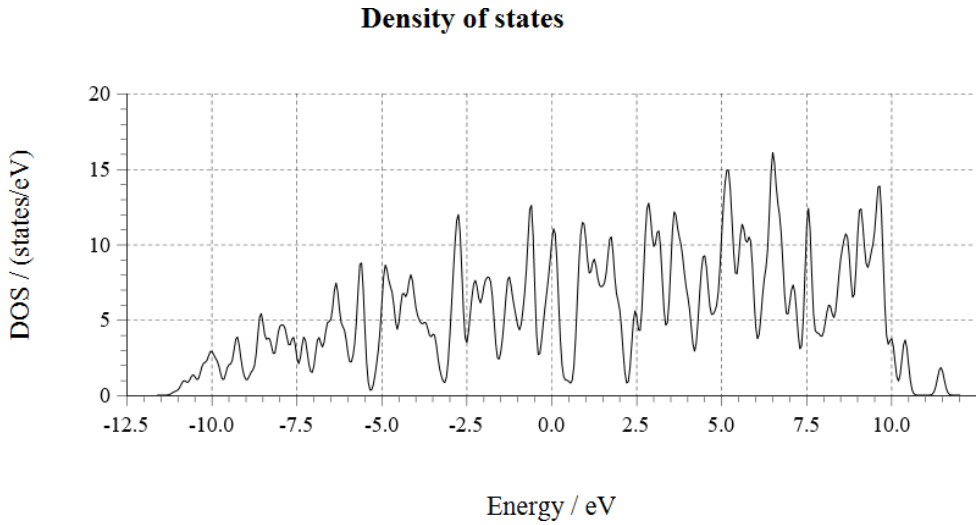


Fig.4:- Density of states of Al wire

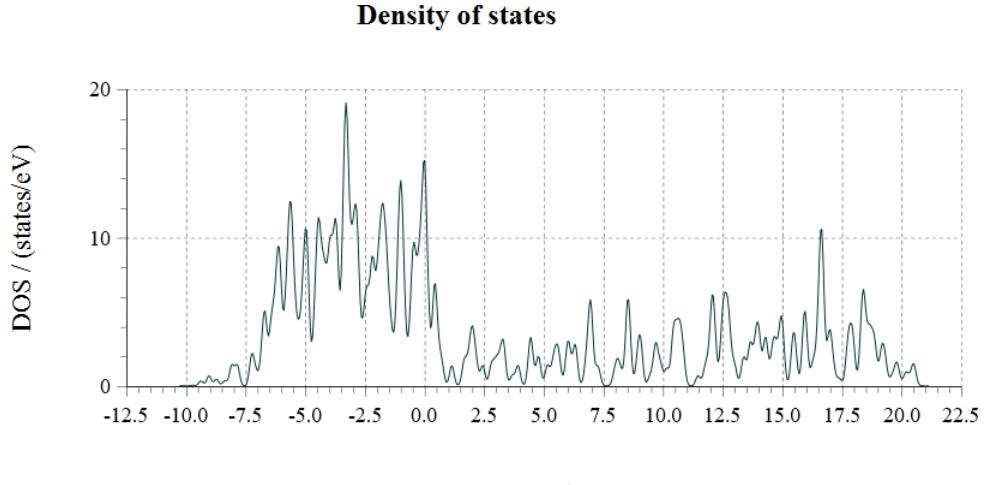
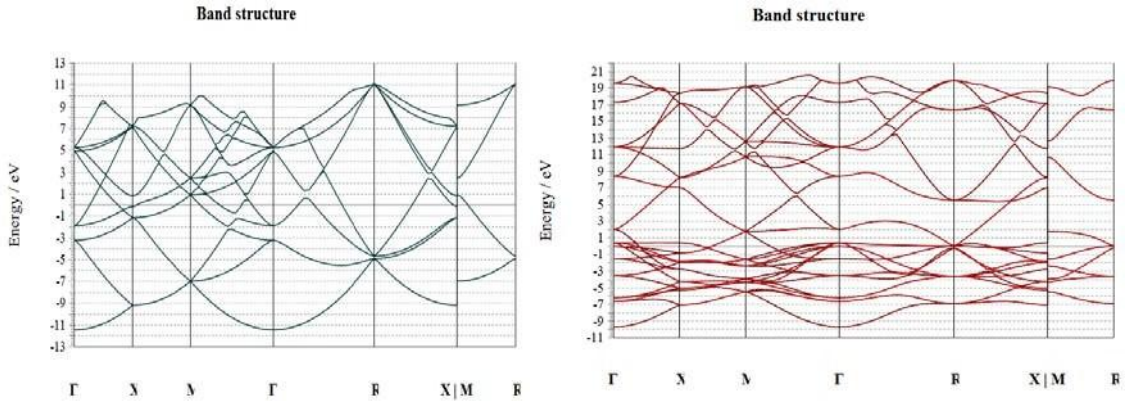


Fig.5:- Density of states of Pt wire

Band structure describes the quantum-mechanical behavior of electrons in solids. Inside isolated atoms, electrons possess only certain discrete energies, which can be depicted in an energy-level diagram as a series of distinct lines. The band structure of Al and Pt wires has been calculated which are shown in figure 6.



(a) (b)

Fig.6:- Band structure of Al and Pt wire

IV. Conclusion

To conclude, we have conducted an investigation on the structural and transport properties of Al and Pt wires using first principles calculations and we compare our result with available previous theoretical data and it can be clearly seen that this current results of the work are in good agreement with the reported results. The values of total energies and fermi energies for Al and Pt wiresare -64.84476189 Ry, -1066.0574 Ry, 8.2690 eV and 16.78eV respectively.

Acknowledgement

The authors are thankful to CNMRL – Indian Institute of Information Technology, Allahabad for providing infrastructural facilities for computational work.

References

[1] Joy L K, Thomas S and Anantharaman M 2016 J. Magn. Magn. Mater. 398 174
[2] Pan F, Song C, Liu X, Yang Y and Zeng F 2008 Mater. Sci. Eng. R-Rep. 62 1
[3] Muhammady S, Kurniawan R, Nurfani E, Sutjahja I M, Winata T and Darma Y 2016 J. Phys.:Conf. Ser. 776 012018
[4] Nie K Y and Hu Z H 2017 Mater. Res. Express 4 065009
[5] Muhammady S, Nurfani E, Kurniawan R, Sutjahja I M, Winata T and Darma Y 2017 Mater.Res.Express 4 024002 Yong Z et al 2016 Phys. Rev. B 93 205118
[6] Ghosh S and Basak D 2017 RSC Adv. 7 694
[7] Muhammady S, Sutjahja I M, Rusydi A, Winata T, Takase K and Darma Y 2017 Jpn. J. Appl.Phys. 56 121201
[8] Fernández Gavela A, Grajales García D, Ramirez J C and Lechuga L M 2016 Sensors 16 285
[9] Chuang C-H M, Brown P R, Bulović V and Bawendi M G 2014 Nature Mater. 13 796

[10] Srivastava A, Sidler M, Allain A V, Lembke D S, Kis A and Imamoğlu A 2015 Nat. Nanotechnol.10 491
[11] Ghoshal T, Maity T, Senthamaraikannan R, Shaw M T, Carolan P, Holmes J D, Roy S andMorris M A 2013 Sci. Rep. 3 2772
[12] Aji A S, Nugraha M I, Yudhistira, Rahayu F and Darma Y 2011 AIP Conf. Proc. 1415 196
[13] Ekomasov A, Stepanov S, Zvezdin K and Ekomasov E 2017 Phys. Met. Metallogr. 118 328
[14] Van Thiem L 2017 J. Electron. Mater. 46 3518
[15] Kondo T, Miyazaki H, Nishio K and Masuda H 2011 J. Photochem. Photobiol. 221 199
[16] Diguna L J, Darma Y and Birowosuto M D 2017 J. Nonlinear Opt. Phys. Mater 26 1750029
[17] Makihara K, Kato T, Kabeya Y, Mitsuyuki Y, Ohta A, Oshima D, Iwata S, Darma Y, IkedaMand Miyazaki S 2016 Sci. Rep. 6 33409
[18] Lee W, Han H, Lotnyk A, Schubert M A, Senz S, Alexe M, Hesse D, Baik S and Gösele U2008 Nat. Nanotechnol. 3 402
[19] Wang D, Liu L, Kim Y, Huang Z, Pantel D, Hesse D and Alexe M 2011 Appl. Phys. Lett.98243109
[20] Yamaguchi T, Shimizu T, Morosawa Y, Takase K, Chen T-L, Lu S-M, Chien H-C and Shingubara S 2014 Jpn. J. Appl. Phys. 53 06JF10
[21] Shimizu T, Aoki K, Tanaka Y, Terui T and Shingubara S 2011
23] Borup R, Meyers J, Pivovar B, et al. Chem Rev 2007;107:3904 – 51.
[24] Yousfi-Steiner N, Mocoteguy P, Candusso D, et al. J Power Sources 2009;194:130– 45.
[25] Wahdame B, Candusso D, Franc ̧ois X, et al. Int Hydrogen Energ 2009;34:967– 80.
[26] Gubler L, Scherer GG. Desalination 2010;250:1034– 7.
[27] Lubitz W, Tumas W. Hydrogen: an overview. Chem Rev 2007;107:3900 – 3.
[28] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, Davide Ceresoli, G.L.Chiarotti, M. Cococcioni, I. Dabo, A.D. Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, Anton Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, Stefano Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A.P. Seitsonen, A. Smogunov, P. Umari, R.M. Wentzcovitch, QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials, J. Phys.: Condens. Matter. 21 (2009) 395502.
[29] D. Vanderbilt, Soft self-consistent pseudopotentials in a generalized eigenvalue formalism, Phys. Rev. B. 41 (1990).
[30] J.P. Perdew, K. Burke, M. Ernzerhof, Generalized Gradient Approximation Made Simple, Phys.Rev. Lett. 77 (1996) 3865–3868.
[31] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu, The Journal of Chemical Physics.