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Investigation of electronic and optical properties of Silver by using Density Functional theory with PBE and WC functional

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ABSTRACT

In this research the electronic and optical properties of Silver such as the real and imaginary part of dielectric function, optical conductivity, energy loss function, extinction coefficient and band structure are calculated. The calculations are done in the framework of Density Functional theory by using Linearized Augmented Plane Wave (LAPW) method and the Generalized Gradient Approximation (GGA). For calculations we used PBE and WC functional that it is corrected version of basic PBE functional. The aim of this work is to compare difference between two PBE and WC functional on electronic and optical properties of silver. Calculated results are in good agreement with previous experimental results.

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INTRODUCTION

Silver lustrous transition metals, it possesses the highest electrical conductivity of any element and the highest thermal conductivity of any metal. The metal occurs naturally in its pure, free form (native silver), as an alloy with gold and other metals, and in minerals. Electronic properties of silver in the experimental work Lewis and Lee (P.E. Lewis and P. M. Lee, 1968) and Christensen (N.E. Christensen, 1972) has been investigated. Silver has Fm-3m group symmetry. Silver is used in reflecting infrared layers in optic pieces like low-emission glasses and sunlight control systems for temperature maintenance and retrieval or for mirrors with high reflection power (R. Dannenberg, 2000), (M. Del Re, 2002), (M. Jamshidnejad, 2011), (J. Mashaiekhy, 2010). Silver is the metal having the highest reflectivity for more than 96% of mirrors solar concentrators is the best choice (P. Nostell, 2000). Silver and its compositions have recently applications in extra-large integrated circuits (M. Jamshidnejad, 2011). Recently the calculations of optical and electronic properties by DFT method is investigated by researchers on silver nano layers, in this work we used DFT method for bulk silver material (S. Hamedi, 2012), (J. Sancho-Parramon, 2010), (G. J. Lee, 2008).

1.Calculation method:

This paper calculations in the framework density functional theory (DFT) using the generalized gradient approximation (GGA) and linearized augmented plane wave (LAPW) with WIEN2k package have been done (Z. Wu and R. E. Cohen, 2006), (J.P. Predew, 1996). In these calculations, the two PBE (Z. Wu and R. E. Cohen, 2006) and WC functional have been used in several studies to obtain lattice constant in solids (J.P. Predew, 1996), (F. Tran, 2007), (J.P. Predew,1992), (R. Dannenberg, 2000). The muffin-tin radius for silver at 2.4 a.u. have been considered. To calculate the number of points 3107 is considered for the classification based on the wave vector Brillouin zone are created. This Divided in three directions 50×50×50 have been considered. To separate capacity states from core states, we selected 6D Rydberg energy. Lattice constant after optimization is 4.122 Å for the PBE functional and 4.048 Å were obtained for the WC functional. The iteration process was repeated until a charge convergence to 0.0001 was achieved. Electronic and optical properties have been calculated for the optimized structure. In Table 1 the optimized lattice constants and the function of the previous research work has been published.

Table 1: results of optimized lattice constant (Å)

Kind of Approximation	Present work	Other's work(Philipp Haas,2009)	Experimental(Philipp Haas,2009)
PBE	4.122	4.152	4.062
WC	4.048	-	4.062

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RESULTS AND DISCUSSIONS

2-1 Band structure:

The investigation of electronic band structure of cubic Ag is very useful in understanding the electronic and optical properties of the material better. Figure 1 shows electronic band structure of Silver that is obtained by using the WC functional, and a diagram of the experimental work (N. E. Christensen) has been added for comparison. In the figure, the lines represent experimental diagram that is in good agreement with obtained results in this study.

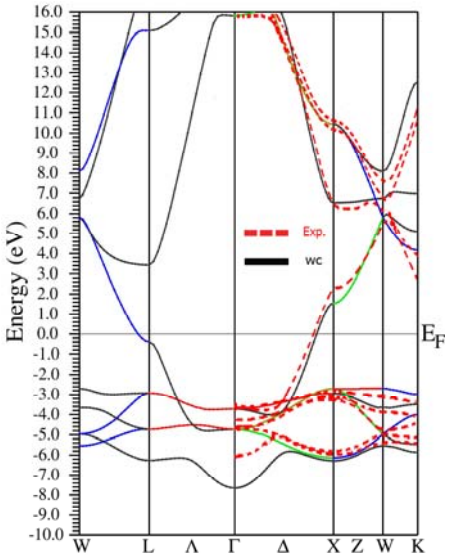

Fig. 1: Electronic band structure of silver by using WC function and experimental results.

2.2 Density of state (DOS):

In density of states diagram the zero energy shows Fermi level and is below the Fermi level and tape capacity by gap energy of the conduction band above the Fermi level for metals and conductive material are separated but have no band gap energy. In Figure 2, the density of states obtained by the PBE and WC functional were compared. The above results indicate that marked noticeably changes low energies, whereas both functional lead to the same results.

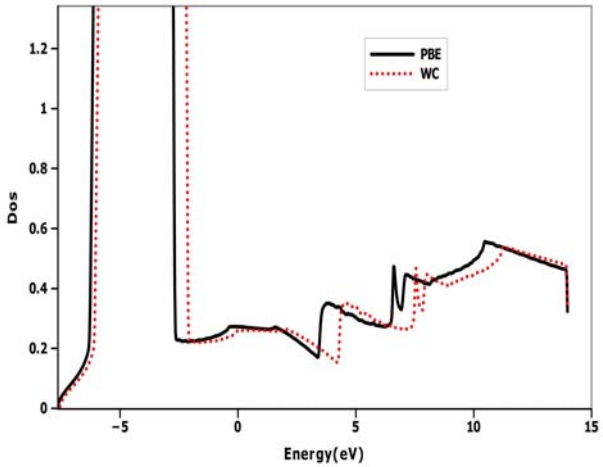

Fig. 2: Density of states (DOS) by using WC and PBE functional.

Dielectric function:

Dielectric function is a complex function of the response electromagnetic field is applied to it. The dielectric function has two inter-band and intra-band components, that inter-band part is used for metals. This function is also shown to be.

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$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \quad (1)$$

Changes could be obtained based on Kramers-Kronig transformation when are available. roots have physical concepts and in fact are the requirement for volume plasmons in the material, while the existence of energy loss is the requirement for the existence of these roots. Also, waves are not propagated and processes of absorption and loss do not take place when is negative.. Here the real and imaginary parts of the dielectric function to separate the two functions are compared. Because the silver face centered cubic (FCC) is changes in both x and z direction is the same. Figures 3 and 4 are shown the changes. PBE and WC have two functional results and high frequencies are almost identical, only one of the other figures in the line frequency is displaced.

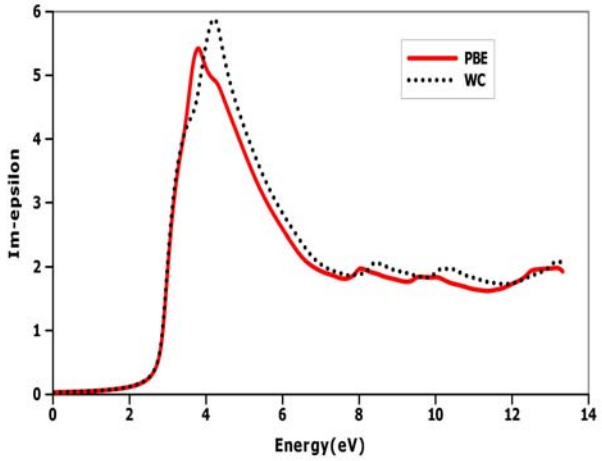

Fig. 3: Imaginary part of dielectric function by using WC and PBE functional.

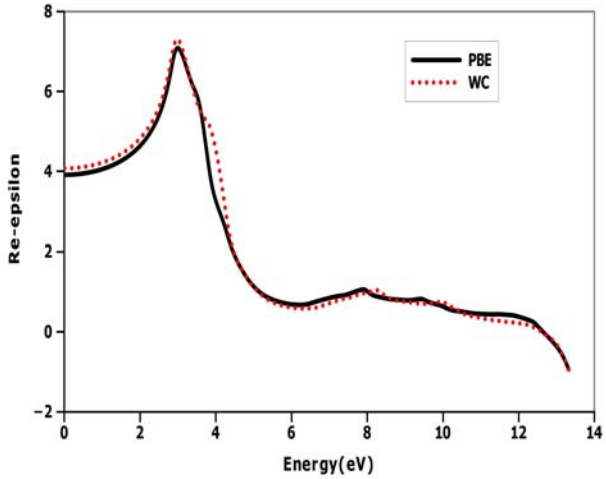

Fig. 4: Real part of dielectric function by using WC and PBE functional.

2.4 refractive index and extinction coefficient:

Optical reflectivity can be calculated from the following equation:

$$R_{\alpha\beta}(\omega) = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \quad (2)$$

Refractive index is a complex function the real part of the n and k characteristic feature is the imaginary part of the index is the extinction coefficient. Figure 6 shows the change in extinction coefficient using the results of calculations based on the PBE and WC functional. According to Figure 6, the small energy region, the extinction coefficient is small and the peak is the same in both graphs. Both values of two functional are consistent with the increase in frequency is slightly less.

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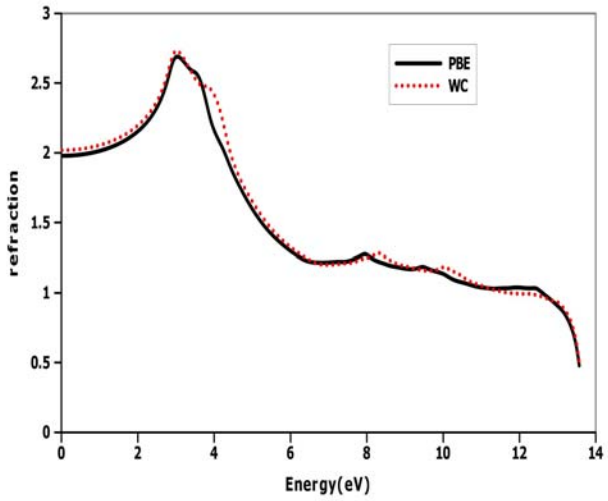

Fig. 5: Refractive index of silver by using WC and PBE functional.

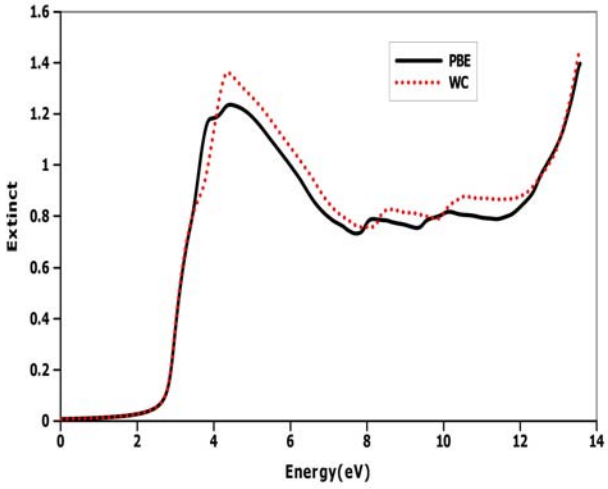

Fig. 6: Extinction coefficient of silver by using WC and PBE functional.

2.5 Energy loss function:

Energy less function is calculated from the following equation:

$$L_{\alpha\beta}(\omega) = -\mathrm{Im}\left(\frac{1}{\varepsilon_{\alpha\beta}(\omega)}\right) \quad (3)$$

The energy loss function can be used to study the electronic structure of matter. The Energy-loss functions describe energy loss of fast electrons transfer the material. The calculated energy-loss function for volume shows intense maximum peaks because of excitation of plasmons. The sharp maxima in the energy-loss functions are associated with existence of plasma oscillations or the energy ħω of volume and surface plasmons. In the average energies, energy loss is depended to the excitation energy of a single electron and electron collective excitation (plasmons). The peak values of volume loss coincide with one of zero values of real part of dielectric function. The peaks of the loss function L(ω) represents a characteristic associated with the plasma resonance, so the corresponding frequency is the so-called plasma frequency. The peak (plasmon energy) by using the PBE functional equal 11.314 eV and 11.870 eV for the WC functional is obtained.

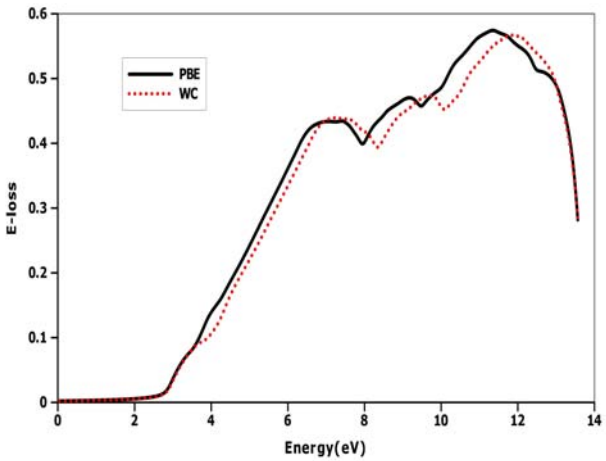

Fig. 7: Energy loss function by using WC and PBE functional.

Conclusion:

In this paper the electronic and optical properties of silver with two PBE and WC method within the generalized gradient approximation in density functional theory framework is used. Electronic and optical properties of the two functional results are not much different. At low energies graphs of the dielectric function, the energy loss function, the density of states and band structure at the charts almost coincide, but at higher energies the function of the WC towards the graph of energy moved slightly PBE are. Finally, the best correspondence between empirical and theoretical results belongs to WC functional.

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