# Study of Lennard-Jones Potential at 300K between Carbon, Silver, Gold and Oxygen Atom

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_Abstract_— The major goal of this study is to look at the Lennard-Jone's Potential (LJP) of different atoms and molecules as they interact. For this, we develop a mathematical model and compute developed model using MATLAB to investigate the Lennard-Jones Potential direct correlation function (LJPDCF) of different atoms/molecules interactions. The carbon-carbon, carbon-oxygen, oxygen-oxygen, water-water molecule, silver-silver, gold-silver, gold-carbon, and silver-carbon interactions were studied for this article. As a result, we discovered that the silver-silver interaction has a maximum LJP of -133.75 kcal/mole at a distance 3.5 Å and a minimum potential of -2.08 kcal/mole at distance 3.8 Å for the carbon-carbon interaction. We discovered a maximum LJPDCF of $3 \times 10^{20}$ in the silver-silver interaction at a distance of 3.8 Å and a minimum Lennard-Jones Potential direct correlation function of $0.25 \times 10^{19}$ in the carbon-carbon and carbon-oxygen interactions at 300K at the same distance of 4 Å. This research could aid in the understanding of the interactions between the considered atom and other atoms in various fields of molecular physics, computational chemistry, molecular models, etc.

_Keywords_— Direct Correlation, Lennard-Jones Potential, Interaction

## I.  INTRODUCTION

The interphase mass and energy transfer phenomena of evaporation and condensation at the liquid/vapor interface are frequent but poorly understood. In order to study these processes at the molecular level, large-scale molecular dynamics simulations of Lennard-Jones (LJ) fluids composed of monomers, dimers, or trimers have been reported in the literature. With strong evaporative cooling and a density differential in the liquid domain close to the liquid/vapor interface, it is discovered that the evaporation rate of LJ monomers in touch with a vacuum is rather high. When the link structure is shortened to just dimers, the rate of evaporation is significantly decreased. Measurements are made of the evaporation and condensation coefficients as well as the velocity distributions of molecules that have evaporated, and the results are compared to those predicted by a model that is already in use and is based on the kinetic theory of gases.

Several elements, including how to establish physical quantities and appropriate parameters to utilize in functions or numbers in simulation input, must be taken into account while producing materials using computational methods. One factor that must be taken into account is the potential for atom interactions in materials. Some of the most frequently used atomic interactions are the Morse, Buckingham, Gupta, LJ, and other potential interactions. Researchers routinely utilize the LJ equation to forecast the characteristics of materials. The LJP can be used to realize interactions among pairs of neutral atoms and molecules in a material system. The parameter values of the atom-to-atom interaction potential are expressed as functions or potential equations. These values can be calculated theoretically (using quantum mechanics), but they can also be confirmed using (classical) simulation, which may then be used to fit experimental data. Physical qualities of a material can be anticipated through simulation by tracking the movement of material atoms inside a molecular dynamic's simulation.

According to Cheng et al., when processes are close to balance and less than one, the evaporation and condensation ratios of both monoatomic and polyatomic molecules are similar and decrease with increasing temperature. Contrary to the conventional belief that these two coefficients are close to unity for monatomic molecules and drop for polyatomic molecules, they are higher for LJ dimers and trimers than that for monomers at the same reduced temperature T/Tc. The data for the two coefficients also combine into a master curve when

displayed against with a translational length equal between the liquid and the vapor phases [1].

The Green-Kubo fluctuation-dissipation theorem was used to calculate the thermal conductivity of solid Argon. In both the NVT and NPT ensembles, separate codes were written to simulate Argon. The atomic dynamics are modeled using the LJ 6-12 potential. The Green-Kubo formalism was discovered to be appropriate for determining thermal conductivity in solids. The Green-Kubo method can be used to determine thermal conductivity in solids. Argon at high temperatures is well represented by hard sphere contacts, which may be computed using a low-cost pairwise force computation rather than more precise but more expensive potentials. This is significant since the Green-Kubo approach necessitates extensive run periods in order to get accurate data. Inui looks at how particles trapped between flat and step-shaped substrates modify their layered structure. The Monte Carlo approach is used to calculate the density profiles of argon atoms interacting with a LJP close to a silicon step. Despite the small spatial changes in the layered structure of the neighboring layer across the step edge, they have an uneven influence on the substrate [2].

The LJ 12-6potential is one of the most extensively utilized intermolecular potentials in classical many-body simulations. In Molecular Simulations, the LJ 12-6 potential is likely the most extensively utilized pair potential. LJ potential is defined as follows:

$$U(r) = k\varepsilon \left[ \left(\frac{\sigma}{r}\right)^n - \left(\frac{\sigma}{r}\right)^m \right] \tag{1}$$

Here k is stand for proportional constant, and are the potential parameters. Particularly for n = 12, m = 6 and k = 4 equation (1) become

$$U(r) = k\varepsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right] \tag{2}$$

The potential between atoms or molecules pairs will be supported by equations (1) and (2). On the basis of fitting experimental data, type of atom values can be estimated. We need cross-interaction potential parameters because we have two different types of atoms. The cross-interaction parameters are [3], according to the popular Lorentz-Berthelot mixing formula, $\sigma$ and $\varepsilon$ is defined as,

$$\sigma_{AB} = \frac{\sigma_{AA} + \sigma_{BB}}{2} \tag{3}$$

$$\varepsilon_{AB} = \sqrt{\varepsilon_{AA} \times \varepsilon_{AA}} \tag{4}$$

Assuming the additivity of atomic potentials and the combination rules for unlike pairings, the energy parameters in the LJ 6-12 potential between atoms (hydrogen, oxygen, nitrogen, and carbon) were calculated using the second virial coefficients of diatomic gases and methane. The relationship allows for the selection of suitable atom parameter settings that replicate the experimental virial coefficients. Due to a divergence in the simple additivity of atomic interactions, the values obtained from the virial data of $H_2$ deviate from those obtained from $CH_4$ [4]. To determine the intermolecular

potential between argon molecules, we used the 12-6 LJP function:

$$U_{Ar}(r) = 4\varepsilon_{Ar} \left[ \left(\frac{\sigma_{Ar}}{r}\right)^{12} - \left(\frac{\sigma_{Ar}}{r}\right)^6 \right] \tag{5}$$

Here $\sigma_{Ar}$ for argon is 0.3405 nm, $\varepsilon_{Ar}$ for argon is $1.635 \times 10^{-21}$J, and r is separation distance of two argon molecules. The (n-6) LJ in term of temperature is derived by Hohm et al. as,

$$U(R, T) = \frac{\varepsilon(T)}{n-6} \left[ 6 \left(\frac{R_m(T)}{R}\right)^n - n \left(\frac{R_m(T)}{R}\right)^6 \right] \tag{6}$$

Here R is distance between two molecules center of mass; $R_m(T)$ is distance at stable condition; $\varepsilon(T)$ is temperature dependent depth and n is the repulsive parameter. Temperature has little effect on the noble gases. The distance between two molecules is measured in nanometers.

$$R_m(T) = R_m(T = 0K) + \delta_0 . f(T) \tag{7}$$

Here, $\delta_0 \cdot f(T)$ denotes the effective increase of molecule size due to vibrational excitation and $f(T)$ is vibrational partition function, $\delta_0$ is temperature independent constant. The potential well-depth is defined as the ratio of temperature independent radius with dependent between two molecules.

$$\varepsilon(T) = \varepsilon(0) \left[ \frac{R_m(0)}{R_m(T)} \right]^6 \tag{8}$$

The objectives of this work are to study the LJ potential for Carbon, Silver, Gold and Oxygen at room temperature. This is important because these elements compounds and material are widely applicable. In this work we study only the bonding strength of one with other like carbon to silver, silver to oxygen, etc. The study of the LJ potential can help to replace the one atom by another if the strength is equal. Several nanoparticles of gold and silver in nanotechnology now a days but the atomic interaction with one another is studies by LJ potential. To prepared the numbers of reagent are used among them oxygen rich reagent is very common. In addition, LJ is also important for investigated monomer model fluid in molecular simulation, testing new theories and simulation methods, for mixtures, phase changes, non-equilibrium phenomena, and interfaces between phases, development of many state-of-the-art force fields for complex molecules, thermodynamic properties, more complex fluids like polymers, electrolyte solutions, and associating fluids. These all are base on binding interaction between the atoms therefore it is necessary to study the LJ potential.

## II. RELATED WORK

In light of our model's maximum temperature of 1100 K [6], this assumption seems tenable. Analytical formulae for the zero-point vibrational energy, anharmonicity modifications of the cohesive energy, and the mode

        

Gruneisen parameter in the Einstein model are derived for the cube lattices (SC, BCC, and FCC) and the hexagonal approach that combines structure. This expands on the work of Wallace from 1965, Corner from 1939, and Lennard Jones and Ingham from 1924. These make use of three-dimensional lattice sums, which can be precisely obtained by converting them into rapid converging series using a variety of expansion techniques. These novel lattice sum methods can be utilized to calculate the critical points for rare gas solids [7].

For modern nuclear reactors, the lead-bismuth non - deposit has long been acknowledged as a potential coolant option. It is also well known that contact with hot, molten lead-bismuth eutectic causes the reactor's fuel cladding to suffer severe damage. Understanding, regulating, and reducing the corrosion process is necessary for both safety and financial reasons. Building a stable oxide scale on the surfaces of structural elements while maintaining the necessary level of dissolved oxygen in the lead-bismuth austenite cooling is one method of preventing corrosion in order to prevent the direct dissolution of metal components. It has been determined how pressure and temperature affect the atomic oxygen diffusion coefficients in $O_2$, $N_2$, Ar, and He as well as the atomic nitrogen diffusion coefficients in $N_2$. The computed collision sizes for atomic oxygen and nitrogen rigid spheres at 280 K are 2.65 Å and 2.75 Å, respectively [8].

Literature found that noble atoms LJ were studies using the two body potentials because the LJ P is so simple, it's great for computer simulations more detail in [9]. The hydrogen bond for hydroxyl-terminated n-alkanethiols is estimated using the following geometrical criteria with O-O separation about 3.5 Å, O-H separation about 2.5 Å, and O-H-O angle ≥120⁰ as per literature assignments modified to the current two-dimensional hydrogen bonded network to explore LJ. The number of hydrogen bonds is determined at each time step and averaged across a minimum of 100 pictures at 300 K [10].

The scientific community is interested in gold nanoclusters because they may have uses in a variety of sectors, such as cancer therapy, medication delivery, biosensing, electronics, and nanophotonic. Plasmon resonance in gold particles is a crucial factor in particular. property has numerous uses, including chemical sensing by cell imaging, catalysis, surface enhanced Raman spectroscopy photoconversion and nonlinear optics. Additionally, gold nanoparticles favorable because to its high level of chemical and physical stability and their bioavailability. As a result, this investigation supports the above-mentioned association of gold nanoparticles with various carbon atoms [11, 12, 13].

The estimated LJP parameters for Ag-C, Au-C, and Ti-C. The depth of the Au-C potential well is almost twice that of the Ag-C interaction. This is consistent with prior DFT simulations using dispersion corrections, which discovered that a gold atom's adsorption energy on graphite is roughly two times higher than a silver atom's [14].

The LJP studies help to studies the differential cross section of shielding materials because the scattering due the atomic binding play an important in radiation shielding. The radiation with suitable wavelength and bond length is consider as perfect shielding materials because it absorbed radiation and protect from different radiation hazard. In addition, LJP also plays an important role for scattering by scattering the radiation when incidence on between two atoms. The interaction of photon in potential cause plays an important role in scattering which is one of the best methods to study the energy, momentum, differential cross section and formation of particles [15, 16, 17].

## III. MATERIALS AND METHODS

The interaction energy U(R) at a fixed point between two molecules of the same kind of atoms can be described as follows using the LJ 6-12 potential:

$$U(R) = \sum_{i,j} \left( \frac{d}{r_{ij}^{12}} - \frac{e}{r_{ij}^{6}} \right) = \sum_{i,j} E \left\{ \left( \frac{2r_w}{r_{ij}} \right)^{12} \right\} - 2 \left( \frac{2r_w}{r_{ij}} \right)^{6} \quad (9)$$

The general LJ potential is provided in equation (1), which has good accuracy for computing simulation results, but the value of k is determined for our research by utilizing equation (10) and taking molecules into account, which sets it apart from previous literature, it was noted that for $n > m$, k is expressed as,

$$k = \frac{n}{n-m} \left( \frac{n}{m} \right)^{\frac{m}{n-m}} \quad (10)$$

Now from equation (9) the intermolecular force can be obtained as,

$$F(r_{ij}) = -\frac{d}{dr} U(r_{ij}) = 6k\varepsilon \left[ 2 \left( \frac{\sigma}{r_{ij}} \right)^{13} - \left( \frac{\sigma}{r_{ij}} \right)^{7} \right] \quad (11)$$

Here first term $\left( \frac{\sigma}{r_{ij}} \right)^{13}$ represent attraction while second $\left( \frac{\sigma}{r_{ij}} \right)^{7}$ represent repulsive. According to Pauli's principle, atoms will resist one other at very near distances. Because of the development of dipole-dipole interactions at a great distance influence Van der Waals force will appear [18]. In addition, LJ potential between two parameters can be calculated using molecular dynamics modeling [19]. The cohesive energy of solid crystal is represented by equation (12) in sluggish gas more detail [20] energy required by solids to divide solids into separate entities for crystals is known as cohesive energy and can be stated mathematically as equation (12). Equation (13) [20] can be used to compute the cohesive energy associated with molecules in a sluggish gas.

$$\Delta E = -(E_g + E_i) \quad (12)$$

      

$$\Delta E = 2N\varepsilon \left[ P_{ij} \left( \frac{\sigma}{r} \right)^{12} - P_{ij} \left( \frac{\sigma}{r} \right)^{6} \right] \tag{13}$$

Equation (13) represented the cohesive energy for a material with an FCC crystal structure with $P_{ij}^{-12} = 12.13188$, $P_{ij}^{-6} = 14.45392$ while for BCC $P_{ij}^{-12} = 9.1142$, and $P_{ij}^{-6} = 12.2533$. In addition, to study the LJP the different parameters of LJP are shown in table 1.

**Table 1:** LJ Potential Parameters

| S.N. | LJP (parameters) | $\sigma$ (Å) | $\varepsilon$ (kcal.mol$^{-1}$) | Reference |
|------|------------------|--------------|----------------------------------|-----------|
| 1. | C-C | 3.3000 | 2.7672 | [21] |
| 2. | C-O(water) | 3.3400 | 3.2284 | |
| 3. | O-O | 0.0100 | 79.2802 | [8] |
| 4. | Ag-Ag | 2.6400 | 183.327 | [22] |
| 5. | $H_2O-H_2O$ | 3.1600 | 4.1969 | |
| 6. | Ag-$H_2O$ | 2.9000 | 27.9030 | |
| 7. | Au-Ag | 0.2647 | 8.8745 | [23] |
| 8. | Au | 0.2646 | 9.5215 | |
| 9. | Ag | 0.2648 | 8.0848 | |
| 10. | O | 3.1660 | 3.5835 | [24] |
| 11. | H | 0.4000 | 1.0608 | |
| 12. | Au-C | 1.7823 | 5.1262 | Calculated |
| 13. | Ag-C | 1.7824 | 4.7296 | |

Direct correlation using mean spherical approximation by Ornstein–Zernike is given as,

$$c(r) \approx -\beta U(r); \quad r > d \tag{14}$$

Here $d$ is the diameter of particles system, $\beta = \frac{1}{k_B T}$, T is absolute temperature of a system, $k_B$ is Boltzmann constant and U(r) is the LJ potential the form equation (14) direct correlation function is obtained as,

$$c(r) \approx -\beta\varepsilon \left[ \left( \frac{\sigma_m}{r} \right)^{12} - 2 \left( \frac{\sigma_m}{r} \right)^{6} \right] \tag{15}$$

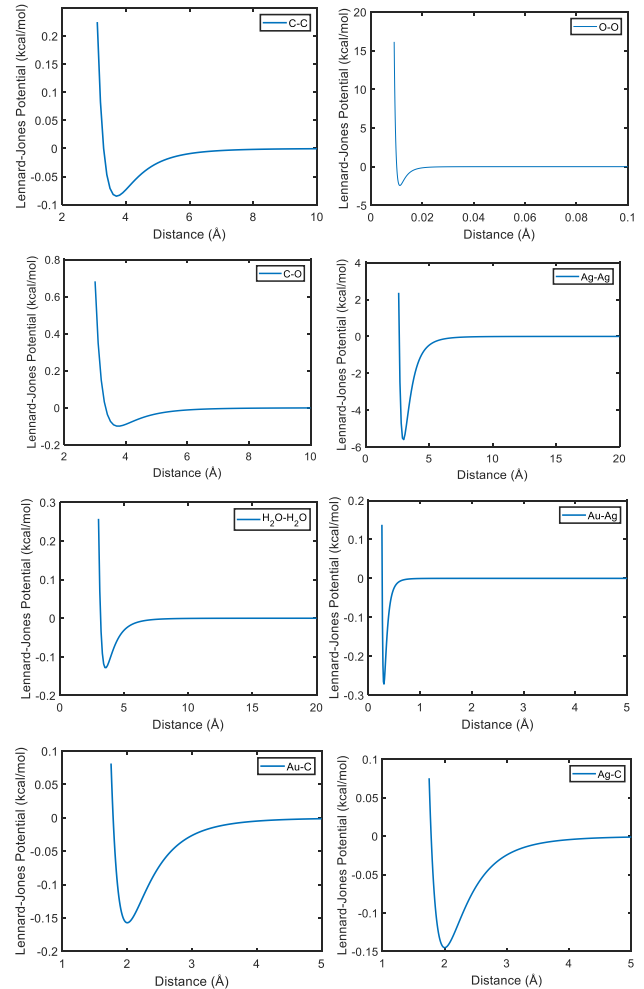At boundary condition radial distribution function is given as,

$$h(r) = -1, r < d \tag{16}$$

For low density system the minimum distance of LJ potential and temperature is related as [25],

$$r_m = \sqrt[6]{1 + \sqrt{1 + (\beta\varepsilon)^{-1}d}} \tag{17}$$

## IV. RESULTS AND DISCUSSION

**Lenard Jones potential with Carbon, Oxygen, Silver, Water and Gold**



**Figure 1:** the variation of Lennard-Jones Potential of interaction of atoms/molecules with the distances.

The above figure 1 shows the variations of the Lennard-Jones Potential of carbon-carbon interaction (C-C), oxygen-oxygen (O-O), carbon-oxygen (C-O), water-water ($H_2O-H_2O$), silver-silver (Ag-Ag), silver-carbon (Ag-C), gold-carbon (Au-C), gold-silver (Au-Ag) with distance separation (Å). Y-axis is the multiplication of 23.06 value. The LJ potential for C-C is gradually increase up to the -1.85 kcal/mol. After the potential reaches to maximum -1.85 kcal/mol, the potential is slowly decreases to the distance 6 Å. After that the potential shows a consistency with increasing the distance. The distance from 3.6 Å to 6 Å, the carbon-carbon interaction of atom shows a broad nature of potential because it ranges from -1.85 kcal/mol to 0 kcal/mol. Study shows the variation of the Lennard-Jones Potential of oxygen-oxygen interaction (O-O) with distance separation (Å), the potential is rapidly increase and become maximum -5.77 kcal/mol at distance 0.01 Å. After that the potential is gradually decrease to the potential zero at distance of 0.02 Å. In shortest ranges of distance from 0.01 Å to 0.02 Å oxygen-oxygen interaction atom shows a constant potential that means narrow nature of potential found.

In the LJ potential for carbon-oxygen interaction of atom shows a broad potential to the distance. The LJ potential is rapidly increases up to -2.3 kcal/mol at the distance of 3.8 Å. After that the potential is gradually decreases to zero at distance 6 Å. The study of LJ potential of silver-silver (Ag-Ag) with distance separation (Å). The LJ potential rapidly increases and become maximum -133.4kcal/mol at the distance 3 Å, after then the LJ potential is gradually decreases with increase of distance. At the distance of 6 Å, the molecules show a constant potential. The consistency in potential after a shortest distance travel from 3 Å to 6 Å. The interaction of water –water molecules show, the LJ potential rapidly increases with distance and maximum – 2.88 kcal/mol at the distance 3 Å, after then decrease from 3 Å to 7 Å and get consistency with increasing the distance. The LJ potential shows a narrow width when gradually decreases from -2.88 to 0 kcal/mol. The study of LJ potential of gold-silver interaction (Au-Ag) shows increase with distance and become maximum -6.46 kcal/mol at the distance 0.2 Å and then after decrease with distance, and become constant.

The study of gold-carbon interaction show LJ potential has width range potential with the distance in Å. The LJ potential is rapidly increases and become maximum -0.16 kcal/mol at distance 2 Å. After that the potential is gradually decreases with increase in distance from 2 Å to 3.5 Å and then show consistency with distance. The study of LJ potential of silver-carbon interaction shows narrow width potential. The LJ potential increases and become maximum -6.46 kcal/mole at distance of 2 Å. The LJ potential is gradually increases from distance 2 Å to 3.5 Å and after then shows consistency with increase the distance. The study of LJ potential of gold-silver interaction shows a very narrow nature of potential and the oxygen and carbon atoms interaction shows a broad nature of potential. The study shows LJ potential of silver-silver interaction shows increase rapidly and become maximum -133.75 kcal/mole at distance 3.5 Å and carbon-carbon interaction have minimum potential -2.08 kcal/mole at distance 3.8 Å, in our studies.

**Spherical approximation for Lennard-Jones potential: Direct correlation function (LJPDCF)**
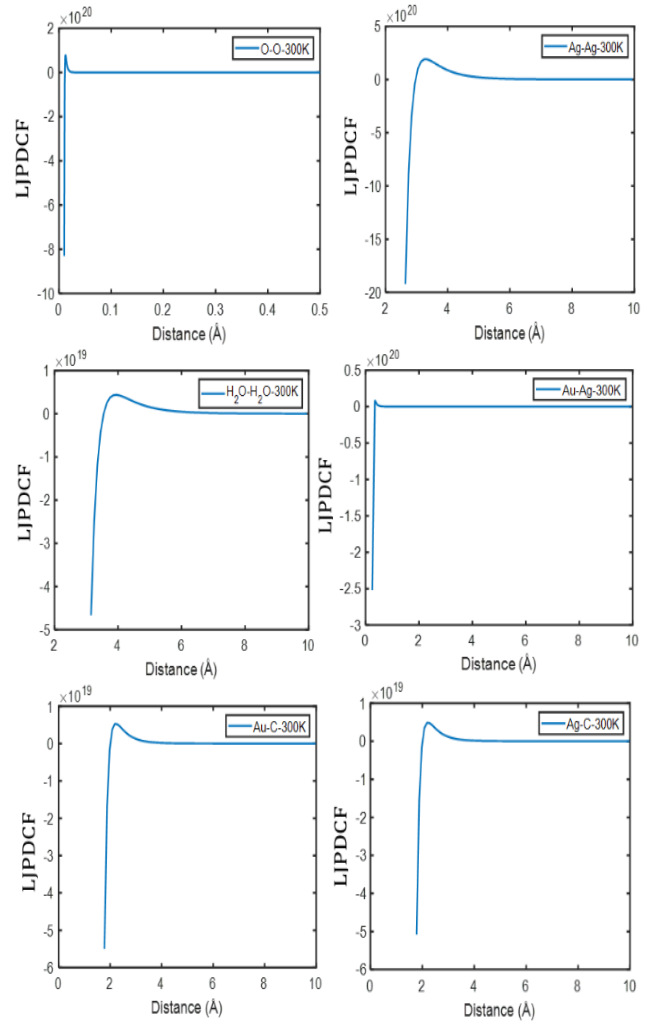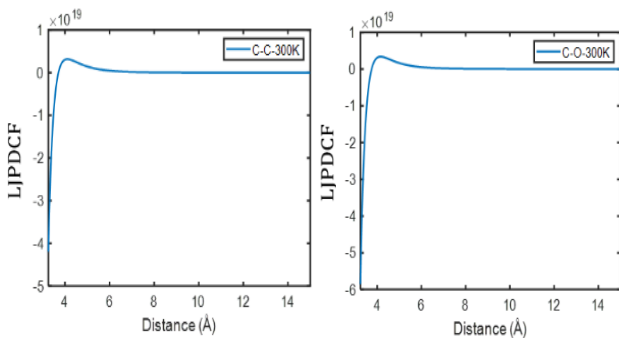




**Figure 2:** The analysis of LJP Direct Correlation function of interaction of atoms/molecules with the distance.

In the above figure, the variation of LJP Direct correlation Function (LJPDCF) of carbon-carbon interaction with distance in A. The correlation function ranges from approximately -4.2 to $0.25 \times 10^{19}$. The maximum correlation function is $0.25 \times 10^{19}$ in the distance 4Å. After the maximum correlation, the function value slightly decreases up to 0 at distance 6 Å. After that consistency in the correlation function with increases of distance. In the variation of correlation function of carbon-oxygen interaction the correlation function gradually increases up to $0.25 \times 10^{19}$ at distance 4 Å. After certain distance the correlation function pick a consistency with increase in distance. The correlation function ranges from -6 to $0.25 \times 10^{19}$. The variation of direct correlation function pf oxygen-oxygen interaction with distance at temperature of 300k, the correlation function ranges from -8.1 to $0.9 \times 10^{20}$. The correlation function sharply increases up to $0.9 \times 10^{20}$ at distance of 0.01 Å. After that correlation function slightly decreases to zero at distance 0.02 Å. After that the function take consistency.

The variation of direct correlation function of silver-silver interaction with distance at 300K, the correlation function

ranges from -19 to $3 \times 10^{20}$. The correlation function is gradually increases up to $3 \times 10^{20}$ at distance of 3.8 Å . After that gradually decreases to zero at distance of 5 Å . The variation of direct correlation function of water-water molecule interaction with distance at 300K, the correlation function ranges from -4.8 to $0.4 \times 10^{19}$. The correlation function is gradually increases up to $0.4 \times 10^{19}$ at distance of 3.8 Å. After that gradually decreases to zero at distance of 5 Å.

The variation of direct correlation function of gold-silver molecule interaction with distance at 300k, the correlation function ranges from -2.5 to $0.1 \times 10^{20}$. The correlation function is sharply increases up to $0.1 \times 10^{20}$ at distance of 0.4 Å. After that sharply decreases to zero at distance of 0.6 Å. The variation of direct correlation function of gold-carbon interaction with distance at 300k, the correlation function ranges from -5.8 to $0.6 \times 10^{19}$. The correlation function is gradually increases up to at $0.6 \times 10^{19}$ distance from 1.8 to 2.2 Å. After that gradually decreases to zero at distance of 4 Å. The variation of direct correlation function of gold-carbon interaction with distance at 300k, the correlation function ranges from -5 to 0. $4 \times 10^{19}$. The correlation function is gradually increases up to at $0.6 \times 10^{19}$ distance from 1.8 to 2.2 Å . After that gradually decreases to zero at distance of 4 Å.

## V. CONCLUSION AND FUTURE SCOPE

The carbon-carbon interaction, carbon-oxygen interaction, water-water interaction, and silver-silver interaction show a maximum potential beyond the distance of 4 Å . Whereas, beyond the distances of 0.02 Å and 0.5 Å, the oxygen-oxygen interaction and the gold-silver interaction both have maximal potential. The gold-carbon interaction and silver-carbon interaction with the same distance 2 Å indicate the common nature of LJ potential throughout the experiment. During silver-silver interaction, the potential has an extremely narrow breadth. The highest Lennard-Jones potential of silver-silver interaction is -133.75 kcal/mole at distance 3.5 Å, while the minimum potential of carbon-carbon interaction is -2.08 kcal/mol at distance 3.8 Å . The carbon-carbon interaction, carbon-oxygen interaction, water-water interaction, and silver-silver interaction all have the same broad nature of LJP Direct correlation function, although the gold-carbon and silver-carbon interactions have the same pattern. The maximum LJP Direct Correlation function of the silver-silver interaction is $3 \times 10^{19}$ at a distance of 3.8 Å, whereas the minimum LJP direct function is $0.25 \times 10^{19}$ at a distance of 4 Å at 300K.

It is important to study the direct correlation function because two-point correlation function or propagators are crucial elements in both classical and quantum models of many-body systems. These two-point functions have a general relation to functional derivatives of a producing functional with regard to two local source terms in functional formulations of many-body theory. The second most abundant derivatives of the free energy, statistical physics of matter, the thermodynamics characteristics of crystalline solids, and the study of hard sphere crystals and their liquid counterparts can all be studied using direct correlation functions. On study the strength of the bond using LJ potential one can used the consider study material for radiation shielding with formation of other elementary particles.

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