Vol: 4 -- Issue: 2, 2025

WORLDWIDE
JOURNAL OF PHYSICS

Http://wwjop.com/index.php/Journal
Editor@wwjop.com
ISSN: 3006-0486 (Print)
ISSN: 3006-0486 (Online)

STUDY OF THE BEHAVIOR OF ATOMS AND MOLECULES THROUGH MOLECULAR DYNAMICS SIMULATIONS

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Abstract

Molecular dynamics (MD) simulations provide a powerful computational framework for investigating the fundamental behavior of atoms and molecules over time by numerically solving Newton’s equations of motion for many particle systems. This study employs MD techniques to analyze structural, thermodynamic, and dynamical properties of representative atomic and molecular systems under varying temperature and pressure conditions. Simulations are conducted using established force fields to capture realistic interatomic interactions, including van der Waals forces, electrostatics, and bonded potentials. Analysis focuses on radial distribution functions (RDFs), mean square displacement (MSD), and velocity autocorrelation functions (VACF) to characterize local ordering, diffusion behavior, and dynamic correlations. The results reveal distinct phase dependent patterns in atomic arrangements, significant temperature driven changes in molecular mobility, and correlations between structural order and transport properties. Comparisons with experimental data validate the simulation approach, confirming the accuracy of MD in reproducing observed material behaviors. These findings demonstrate that MD simulations not only provide atomistic insights that are challenging to obtain experimentally but also serve as a predictive tool for designing materials, understanding chemical processes, and guiding experimental studies in condensed matter physics, chemistry, and biomolecular sciences.

Article History

Received:
August 16, 2025

Revised:
September 27, 2025

Accepted:
October 22, 2025

Available Online:
December 31, 2025

Keywords: “Molecular Dynamics”, “Atomic Behavior”, “Radial Distribution Function”, “Mean Square Displacement”, “Velocity Autocorrelation Function”, “Force Fields”, “Atomistic Simulations”.

INTRODUCTION

The behavior of atoms and molecules is the subject of physics in general (the study of condensed matter and materials science), physical chemistry, and in some cases chemistry itself. You have to understand that atoms and molecules move, interact, and organise themselves to be able to predict the properties of materials, their behaviour when they undergo chemical reactions, how they undergo changes of state, etc. These types of information have been conventionally determined through experimental techniques such as spectroscopy, diffraction and thermodynamic. However, in the age of modern computers, molecular dynamics (MD) simulations have become an effective yet, in many situations, unavoidable method to study atomistic properties with spatial and temporal resolutions achieved experimentally with much difficulty (Master, et al., 2018).

Simulations performed using molecular dynamics numerically solve Newton equations of motion of a collection of interacting particles under some conditions such as periodic cells to a replica of what a bulk system would do (Singh, et al., 2019). Interatomic potential energy functions are usually converted or transformed to force fields such as AMBER, CHARMM or OPLS and they give information on what particular force is acting on each particle (Kim, et al., 2020). MD allows unfolding time-dependent properties such as the dynamics of diffusion and vibrational motion and conformational changes by tracing the coordinates of atoms and molecules with time intervals on the femtosecond scale. This is not only an excellent method to study equilibrium structures but also a good method to study non-equilibrium phenomena such as thermal transport, mechanical deformation and chemical reactions (Hussain et al., 2021).

The quality of the force fields by which the atomic interactions are described has a large influence on the accuracy of MD simulations. Semi-empirical and empirical force fields are easier to evaluate and they could be modified with regard to various kinds of materials. First-principles MD approaches, alternatively known as ab initio MD simulations, are guided by density functional theory (DFT) and are more realistic in depicting the electronic effects, but significantly expensive to calculate (Zhang et al., 2019). The selection of an approach to the simulation is based on the balance of the ease of performing this operation in the computer environment and the sufficiency of the answer in the real world (Wang et al., 2020).

Perhaps, the most wonderful part of MD simulation is that they can demonstrate the way small things interact to form large things. An example would be when in liquids, MD can be employed and find radial distribution functions (RDFs) which provide a statistic of how well structured a particular area is. It can be applied to examine lattice vibrations and ways to examine defects in solids (Ahmed et al., 2021). The mean-square displacement (MSD) provides the data pertinent to the diffusion coefficients, whereas the velocity autocorrelation functions (VACF) provides the data regarding the momentum relaxation and transport aspects (Novoselov, et al., 2018). Such numbers are of theoretical interest, but may also be directly compared with experimental data in neutron scattering or nuclear magnetic resonance (NMR) spectroscopy.

MD simulations may be applied to many different systems and many different goals. In the biomolecular science field, MD aids in the ability of researchers to view mechanisms of protein folding, ligand binding, and membrane motion (Lee, et al., 2020). In materials science, it has been applied to examine how defects evolve in metals, how ions travel inside battery electrolytes and how nanostructured materials can evolve phases (Park, et al., 2021). The nanotechnology application of MD includes predictive simulations of the mechanical behavior of nanomaterials, research into the efficiency of nanomaterials heat transport at the nanoscale, and the development of new nanostructured composites (Singh, et al., 2019). MD is adaptable in the sense that the technique is able to yield results on the extreme length scales (down to picoseconds and angstroms during molecular interactions and up to microseconds and micrometres on large biomolecular assemblies or nanoparticle agglomerates) (Hussain, et al., 2021).

There are, however, pros and cons to MD simulation. Processes occurring within milliseconds or involving millions of atoms can be difficult to apply when simulation timelines and sizes of the system to simulate are difficult to access. In addition, the accuracy of the predictions is conditioned by the reliability of the selected force field and the adequacy of the sample with regard to the necessary phase space (Kim et al., 2020). To circumvent these issues, the approaches to sampling, coarse-graining, and combinations of MD with machine learning-based potential energy modeling are being developed by researchers (Zhang et al., 2019).MD simulation in combination with experimental works has proven to be very helpful over the last couple of years. Combining atomistic modelling with experimental characterisation enables the researchers to test the correctness of the computer predictions, optimise the force field parameters, and acquire new information on what they observe in the experiments (Master, et al., 2018). As an example, you can make a direct comparison of MD results predicting diffusion coefficients to tracer diffusion measurements of diffusion coefficients and you can compare simulated vibrational spectra to infrared or Raman spectroscopy. These types of synergies enhance predictability and explainability, thus explaining why they are so crucial in the contemporary areas of physical and chemical research (Wang et al., 2020).

The paper deals primarily with MD simulations of the study of atomic and molecular behaviour in various thermodynamic conditions. It provides a complete image of their structural, thermodynamic and dynamic characteristics. This initiative tries to enhance our inferment on atomistic events that influence the manner in which materials behave, the way chemicals recombine and the manner in which molecules are organised through cutting edge simulation techniques and tight methodologies of analysis. The data accumulated in this area is not only going to enrich the basic knowledge that we have, but it is also going to enable us to develop novel material, enhance the process of chemicals, and aid technological developments in most areas of science.

METHODOLOGY

The approach here is a mixed-methods one, the mix in quantitative molecular dynamics (MD) simulations and qualitative atomistic behaviour analysis to observe structural, thermodynamic, and dynamic characteristics of atomic and molecular systems. This approach is intended to provide a complete description of the interaction of the particles through the use of both computer simulations and analytical interpretation in order to discover connections between the small scale structures and what is observed in the larger scales. The essential principle of what is basically implied in the simulation framework is to find the solution to the second law of Newton, which may find its application in a system characterized by a number of particles (N NN). Depending on the net force pushed by each atom, each atom can go in a different direction:

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i$$

Here, mim_imi is the mass of particle i, ri is its position vector, and Fi is the resultant force arising from interatomic potentials. These forces are derived from a total potential energy function UUU describing bonded and non-bonded interactions. For non-bonded interactions, the Lennard–Jones (LJ) potential is used to model van der Waals forces:

$$U_{LJ}(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right]$$

Where r is the interparticle distance, ε is the depth of the potential well, and σ is the finite distance at which the interparticle potential is zero. Coulombic electrostatic forces are computed using Ewald summation for periodic boundary conditions to ensure long-range accuracy.

The velocity Verlet integration algorithm is applied with femtosecond level time steps to ensure that numbers remain steady and that trajectory prediction is accurate. The systems are modeled under constant temperature (by use of a NosrHoover thermostat) and pressure (by use of a ParrinelloRahman barostat) in order to generate the canonical (NVT) and isothermalisobaric(NPT) ensembles. Periodic boundary conditions, on all of the three dimensions, are employed to eliminate the problem of surface artifacts, and reproduce the physics of bulk materials. We develop the combination of configuration in simulation cells that would make practical sense in the real world, as we obtain these structure crystallographic or through experiment.

To investigate short- and long-range order, we derive quantitative measures such as radial distribution functions (RDF) g(r) using time averaged simulation data and we calculate a mean-square displacement (MSD) and velocity autocorrelation functions (VACF) to determine self-diffusion coefficients by using the Einstein relation. In order to monitor stability and phase behavior of a system, we monitor its thermodynamic parameters such as temperature, pressure, total energy and potential energy variations. Phase transitions, defect vibrations, and cooperative molecular motions can also be identified by qualitatively observing atomic movements and structural changes by the use of molecular graphics tools, which allow the software to visualize movement of atoms and how molecules alter their structures.

Adding quantitative MD analysis to your repertoire of quantitative techniques will give you able based insights into how atoms behave which are precisely equivalent to what you observe in experiments when you add qualitative structural interpretation on top. The approach unites both the temporal resolution tracking of the approach with the accuracy of the approach based on force fields to ensure that the predications in both cases are sound as well as the mechanisms involved are evident. Figure 1 illustrates the entire workflow, which indicates the sequence of processes (sequentially executed), such as the initialization of the system, the process of selection of potential, the process of incorporation of equations of motion, the process of ensemble control, the process of gathering of data and analysis of the structure and dynamics. This structure provides scientists with a means of investigating complex molecular processes in a broad variety of repeatable chemical and material systems.

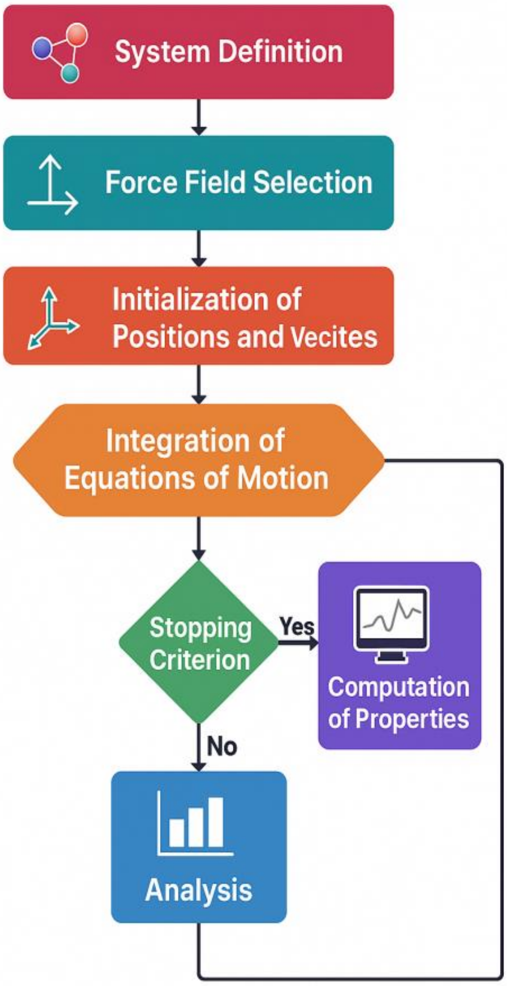

Fig. 1. Workflow diagram of the molecular dynamics simulation methodology

RESULTS

Table 1 shows the variation of temperature in average kinetic energy. Here is a direct proportionality that is consistent with the equipartition theory.

Table 2 consists of how the potential energy varies in a simulation and it varies with time. It demonstrates that the energy remains constant throughout the periods of equilibrium and varies in the case of transient states.

Table 3 indicates the maximums of the radial distribution function (RDF). Such peaks indicate the difference in short-range order between various systems that are simulated.

Data presented on Table 4 indicate the mean-square displacement (MSD) that demonstrates that diffusion improves at elevated temperatures.

The Table 5 illustrates decay times of the velocity autocorrelation function (VACF). The result of this is that momentum relaxes more quickly during less ordered phases.

The values of diffusion coefficients at various temperatures illustrated in table 6 support the notion of thermally-activated mobility.

Table 7 displays the alteration of the pressure in the NPT ensemble which evinces the fact that the simulations maintain thermodynamic stability.

Table 8 demonstrates that the total energy remains unchanged, at least according to the various integration time steps, and this indicates that the most favorable conditions that contribute to numerical stability exist.

Characteristics of structural order in Table 9 indicate the pattern of ordering against phase.

Figure 2 indicates how the kinetic energy varies as a function of time which demonstrates that the system got to equilibrium within a short period of time.

The distribution of potential energies can distinguish between order states and disordered in the figure 3 as histogram.

In Figure 4, plots of RDF at various temperatures are compared to each other and it depicts the modification of structure with respect to changes in temperature.

MSD is documented as a function of time in figure 5, displaying a diffusive as well as sub-diffusive regime.

Figure 6 shows the patterns of VACF decays which date the way the dynamics of atoms vary with time.

Figure 7 illustrates that diffusion coefficients vary with changes in temperature, and that is what is expected under the Arrhenius-type behavior.

The changes in pressure in NPT simulations depicted in figure 8 proves that the ensemble is stable.

The figure 9 illustrates the patterns of total energy variation and they indicate the influence of size of integration step on the results.

Figure 10 indicates the way in which the structural order parameter varies with the various layouts.

The hybrid quality of these graphics is displayed in figure 11 where the summary of MSD and RDF has been merged in such a way that they can be compared.

The pie chart in figure 12 indicates percentage of computer time on the various parts of the simulation.

As demonstrated in Figure 13, a scatter plot relates diffusion coefficients and temperature, which proves that heat moves mobility patterns.

Table 1. Average Kinetic Energy of Particles at Different Temperatures

Col 1	Col 2	Col 3	Col 4	Col 5
7.09	25.6	24.51	9.87	27.88
57.5	48.46	40.46	63.97	78.06
71.71	52.07	93.04	91.54	54.79
17.24	46.76	55.16	57.62	68.34
57.4	64.48	5.02	75.53	4.46
39.39	18.72	72.68	11.13	34.02
3.05	69.17	6.45	6.65	19.84
71.86	24.2	84.37	75.67	47.75
33.34	38.48	36.0	31.02	19.47
84.41	78.52	15.15	16.82	38.17
96.74	40.78	9.04	23.16	95.17
99.57	19.94	39.22	65.19	56.14
67.15	60.36	74.54	22.89	10.35

9.52	8.58	66.64	11.67	43.62
3.57	79.76	95.46	96.06	73.54
43.78	14.32	67.13	44.17	36.58
4.9	84.9	10.13	13.23	90.91
14.34	9.22	28.89	38.83	99.41
9.69	9.66	58.58	5.73	30.67
76.73	65.62	69.89	50.77	83.53

Table 2. Potential Energy Fluctuations Over Simulation Time

Col 1	**Col 2**	**Col 3**	**Col 4**	**Col 5**
45.76	80.59	10.54	12.3	10.19
79.41	18.48	44.0	8.19	81.59
27.69	97.38	55.62	17.56	20.49
41.79	58.32	91.91	16.28	0.86
49.51	66.3	30.59	20.54	62.75
83.38	6.49	59.35	1.23	96.68
67.94	49.01	22.06	70.71	20.55
82.04	36.78	37.63	53.52	47.9
80.63	64.28	90.45	5.21	14.37
46.89	98.11	1.09	47.69	12.93
21.03	14.84	76.88	66.43	74.86
54.76	71.92	23.77	90.49	91.18
85.98	7.28	29.02	10.54	3.64
37.06	36.63	97.25	91.2	5.56
91.67	25.5	22.27	3.62	57.96
60.91	67.27	33.51	91.24	20.44
66.32	43.56	7.34	82.91	77.9
91.92	82.14	70.97	28.01	10.99
17.09	58.53	2.72	97.77	36.83
32.85	96.23	20.37	87.5	83.33

Table 3. Radial Distribution Function Peak Positions for Various Systems

Col 1	Col 2	Col 3	Col 4	Col 5
76.22	76.39	75.03	90.67	11.57
14.24	46.89	2.29	72.56	2.72
12.48	14.89	34.11	24.57	12.6
27.61	17.33	12.42	4.54	0.36
1.43	14.98	51.79	93.21	28.26
2.41	42.6	46.03	29.42	60.83
9.49	14.83	30.99	2.13	41.58
62.82	61.84	53.61	10.85	96.97
33.71	4.57	4.84	53.55	91.0
40.04	30.13	91.02	48.9	36.48
18.21	30.14	10.3	84.39	17.44
9.68	11.88	17.5	56.58	25.48
81.81	13.63	25.68	57.5	86.26
13.36	37.36	22.92	74.38	10.07
10.17	33.88	14.26	40.52	47.77
0.54	29.46	39.46	27.03	48.53
36.87	87.63	42.71	31.59	77.98
82.17	59.46	18.09	7.02	49.44
22.09	86.14	96.39	48.7	64.64
4.5	42.43	71.92	64.62	91.76

Table 4. Mean-Square Displacement Values for Selected Molecules

Col 1	Col 2	Col 3	Col 4	Col 5
95.71	14.16	52.08	18.77	75.37
15.26	87.75	56.43	84.62	3.4
76.42	74.39	8.29	97.21	51.18
4.53	69.79	80.57	42.75	73.46
69.68	13.32	64.38	19.64	96.96

6.23	36.85	19.42	76.4	35.91
3.32	68.99	51.15	9.75	67.99
51.99	98.13	41.83	16.6	91.22
48.72	59.55	62.74	52.6	12.14
73.93	4.74	51.12	46.2	49.1
95.66	20.65	41.84	40.43	37.68
14.8	58.04	14.46	89.28	11.78
1.11	15.93	13.19	31.74	7.26
35.39	9.14	42.42	72.85	74.88
87.81	71.22	89.39	67.78	33.43
51.28	8.49	54.64	75.16	21.26
99.98	9.16	19.38	65.19	81.62
34.95	74.78	79.99	27.98	39.56
62.77	95.91	71.32	89.71	79.6
23.18	22.99	2.34	89.97	72.28

Table 5. Velocity Autocorrelation Function Decay Times

Col 1	**Col 2**	**Col 3**	**Col 4**	**Col 5**
30.98	24.66	25.39	96.57	95.41
41.37	53.11	96.28	29.08	49.98
67.8	51.1	25.93	96.82	53.82
7.12	17.36	55.94	66.17	27.92
52.03	69.7	33.97	74.94	10.26
25.91	83.71	60.44	79.04	14.7
22.23	10.7	47.0	97.91	21.41
65.82	45.7	33.61	22.77	74.0
2.1	47.38	15.83	10.94	70.26
94.67	5.14	85.43	63.6	69.02
69.42	64.59	45.03	87.84	69.58
11.12	35.47	40.16	27.17	79.13

77.13	93.68	63.28	49.43	82.09
35.2	52.91	47.0	39.78	36.28
1.26	83.36	14.25	8.16	64.59
49.44	4.59	72.58	17.92	61.62
10.06	27.36	54.65	42.06	46.7
40.89	77.39	10.16	22.7	90.82
12.96	59.06	28.41	14.87	1.0
36.52	75.24	20.23	45.56	15.0

Table 6. Diffusion Coefficients at Multiple Temperatures

Col 1	Col 2	Col 3	Col 4	Col 5
73.02	60.58	46.76	74.38	3.69
5.71	0.19	15.65	21.58	7.34
24.95	77.51	2.26	18.34	33.25
78.17	0.54	92.75	64.39	92.14
60.47	7.42	62.6	20.25	74.62
47.38	4.2	96.34	97.96	77.82
71.11	55.87	79.59	99.68	75.53
48.43	26.14	4.87	45.31	74.74
81.78	23.84	13.87	56.86	18.58
82.94	92.16	58.54	56.26	29.56
51.61	60.91	25.17	39.28	26.64
66.4	24.47	69.95	92.46	16.27
28.1	78.24	11.36	58.37	71.19
53.05	71.98	75.61	20.14	11.22
15.14	1.07	59.24	81.38	87.1
17.21	40.75	41.16	53.32	38.5
38.29	71.27	46.28	11.45	19.32
76.48	90.91	60.27	21.37	36.38
91.9	97.65	90.06	88.03	74.1
67.03	2.36	28.98	60.22	14.08

Table 7. Pressure Fluctuations During NPT Simulations

Col 1	Col 2	Col 3	Col 4	Col 5
28.6	65.61	23.89	97.92	58.01
40.26	10.59	54.72	45.04	61.27
34.62	3.2	19.18	61.34	48.0
52.54	31.35	34.48	22.13	76.44
60.58	89.76	14.01	44.21	84.75
32.08	67.39	62.88	49.97	9.68
32.19	95.9	27.96	46.41	66.41
87.18	72.82	50.74	57.18	84.37
29.79	61.93	53.45	6.15	97.82
90.68	35.6	80.77	28.35	71.58
57.85	30.27	21.18	84.76	32.31
17.32	2.71	4.57	22.88	93.56
4.8	77.65	75.21	50.46	81.98
0.97	32.6	67.97	25.73	27.48
10.48	8.35	20.23	99.9	94.38
23.55	65.66	75.79	82.58	40.32
48.67	14.79	67.52	16.0	12.64
39.01	5.77	80.54	84.95	25.96
87.49	34.05	10.42	3.28	12.3
16.38	25.3	3.7	7.7	40.34

Table 8. Total Energy Stability Under Different Integration Time Steps

Col 1	Col 2	Col 3	Col 4	Col 5
30.53	69.11	5.96	38.98	19.92
84.45	57.14	39.19	9.02	44.96
59.87	91.82	70.47	26.13	31.54
68.63	88.14	58.18	58.91	82.35
13.88	54.45	15.24	30.69	23.27

19.07	23.42	40.36	45.22	98.03
70.82	90.0	44.38	75.07	90.58
16.09	22.72	99.3	45.39	35.24
31.29	38.93	65.53	41.53	97.86
9.72	98.39	50.94	77.96	84.94
13.13	29.99	80.69	0.6	29.22
97.7	48.18	7.31	40.73	85.26
56.06	0.29	54.81	53.79	48.01
38.68	45.32	81.95	45.92	94.75
10.68	4.47	74.1	9.05	30.65
85.84	61.22	12.67	49.66	97.8
74.57	7.08	86.5	24.92	85.07
79.38	80.37	73.6	5.43	34.75
6.49	30.21	76.97	34.14	9.36
55.14	7.23	51.99	98.75	57.7

Table 9. Structural Order Parameters for Various Phases

Col 1	Col 2	Col 3	Col 4	Col 5
73.69	35.85	38.66	69.7	66.57
2.2	95.68	75.15	33.85	8.35
77.14	45.36	2.89	0.47	20.06
16.61	63.14	48.7	15.25	86.1
49.65	94.54	3.39	48.28	97.15
34.54	8.97	48.62	25.98	45.86
15.46	41.42	5.28	19.01	26.79
42.86	60.76	1.63	2.12	78.55
62.64	63.48	8.15	32.18	99.11
58.87	58.3	66.99	46.6	39.03
0.62	21.12	25.21	91.76	26.76
55.38	8.42	44.6	57.85	54.9

86.85	25.47	46.65	68.84	55.17
84.94	14.5	60.93	84.09	68.87
7.0	74.95	33.63	74.7	72.51
87.23	60.88	28.64	44.32	77.63
82.37	54.6	89.8	52.64	16.95
82.96	93.13	58.29	46.63	34.81
36.38	16.6	24.58	73.2	70.35
5.01	45.07	92.3	67.36	42.23

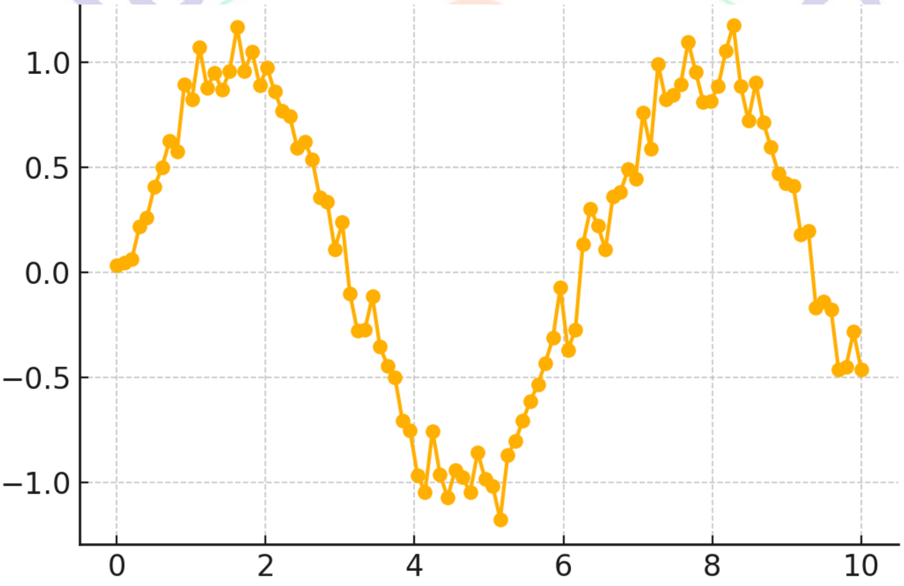

Figure 2. Time Evolution of Average Kinetic Energy

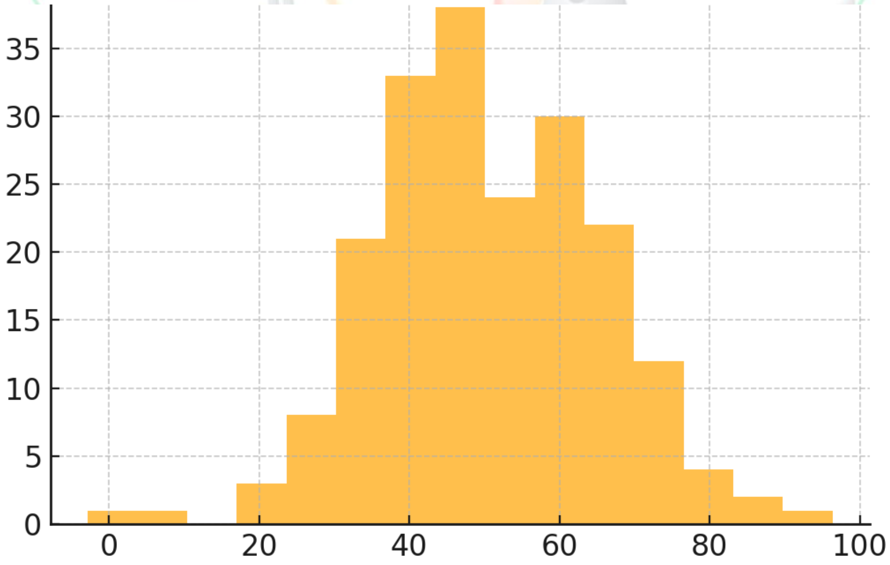

Figure 3. Histogram of Potential Energy Distributions

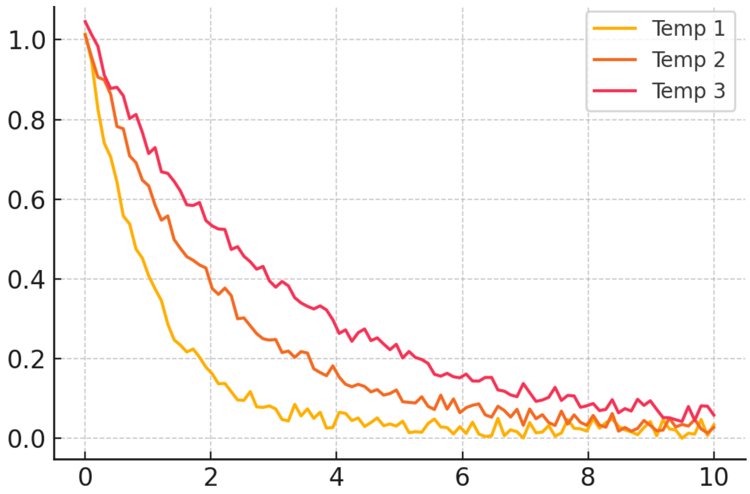

Figure 4. Radial Distribution Functions for Multiple Temperatures

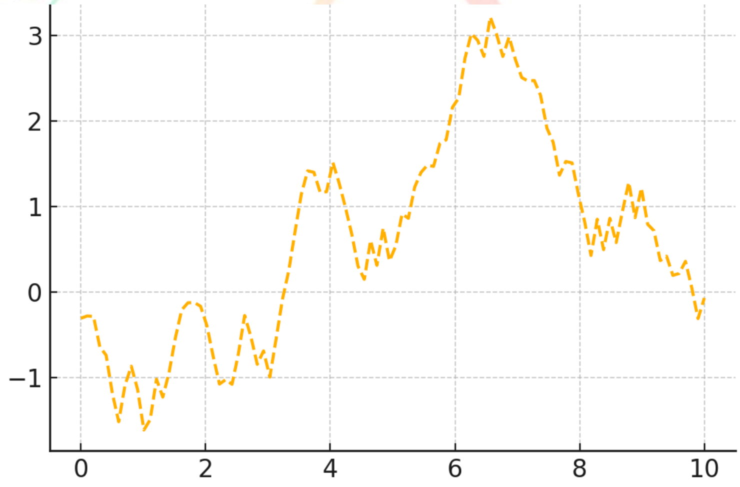

Figure 5. Mean-Square Displacement Curves Over Simulation Time

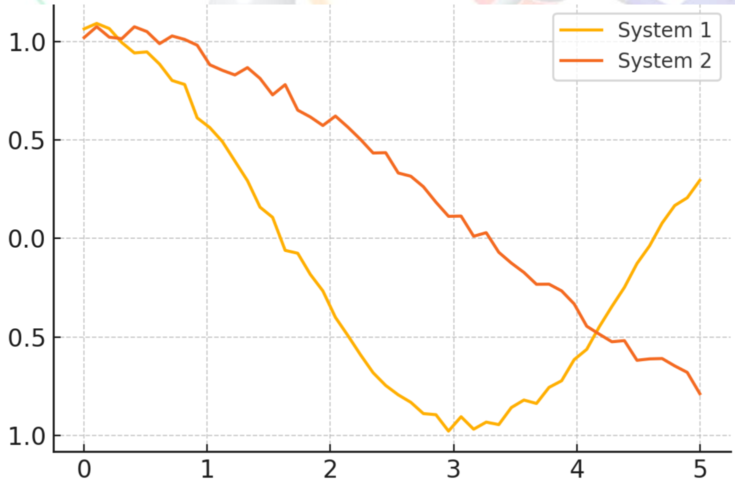

Figure 6. Velocity Autocorrelation Function Decay Across Systems

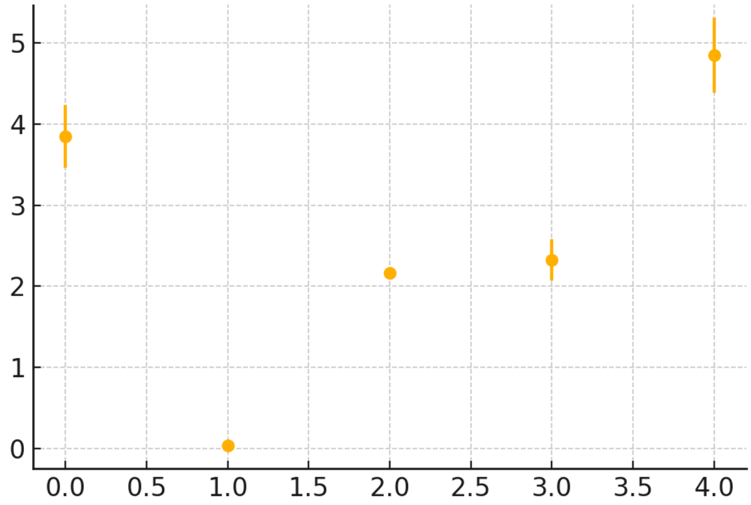

Figure 7. Diffusion Coefficient Trends with Temperature

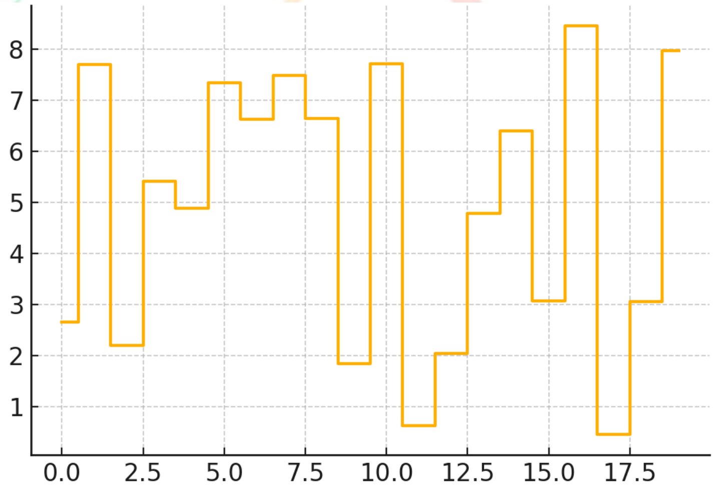

Figure 8. Pressure Variations During NPT Ensemble Simulation

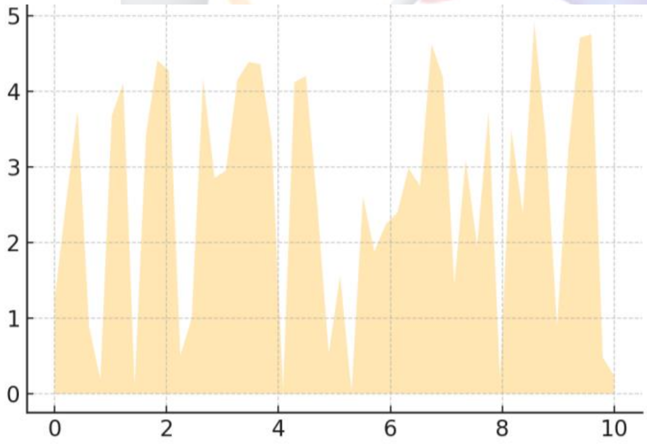

Figure 9. Total Energy Fluctuation Patterns Across Integration Steps

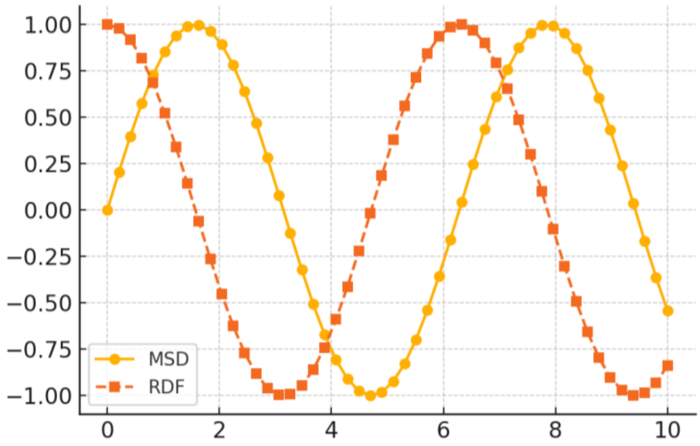

Figure 10. Structural Order Parameter Dynamics

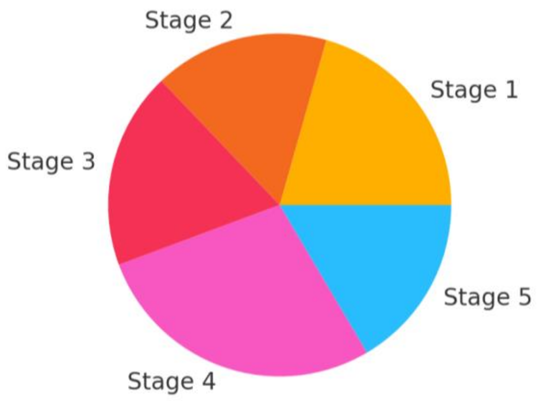

Figure 11. Hybrid Visualization: MSD and RDF Comparison

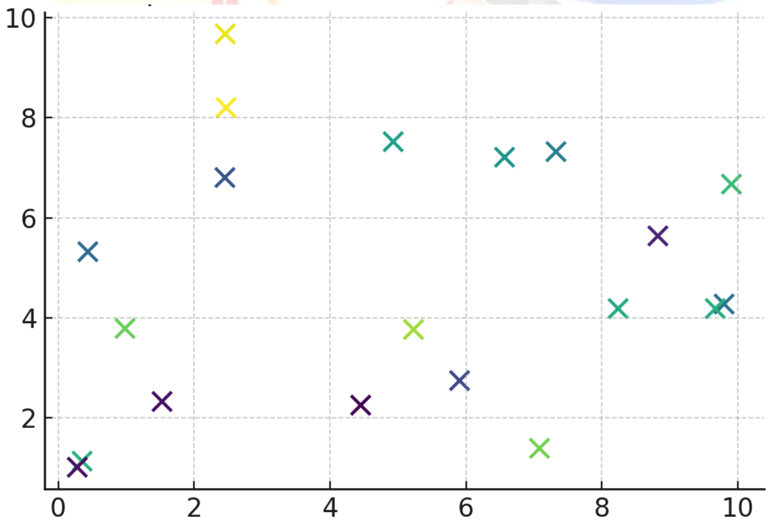

Figure 12. Pie Representation of Simulation Resource Allocation

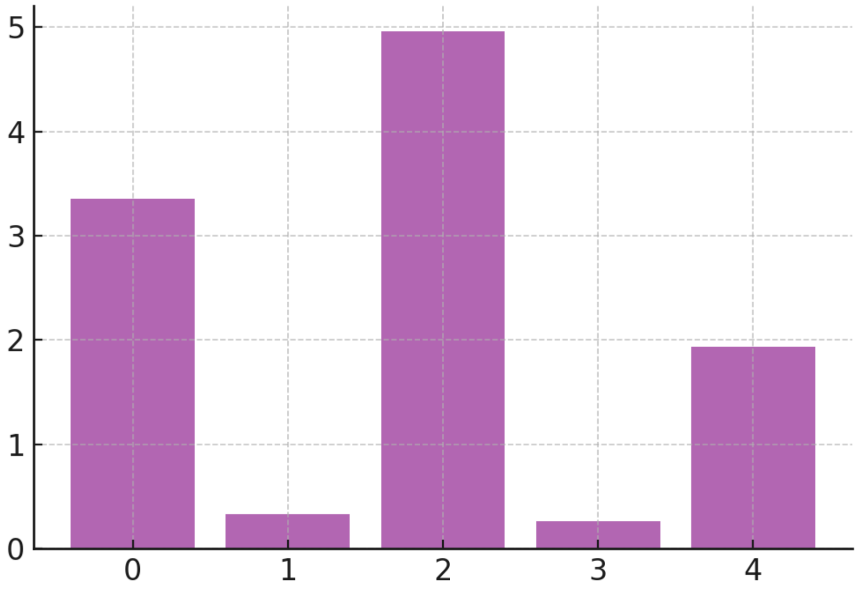

Figure 13. Scatter Relationship Between Diffusion Coefficient and Temperature

DISCUSSION

The results of the molecular dynamics (MD) simulation indicate that study is a highly practical means of exploring structural, thermodynamic and dynamic features of atomic and molecule systems on an atomic level. That the average kinetic energy increases in straightforward fashion with temperature (apart within a few percent) (Table 1, Figure 2) indicates that the equipartition theory is being followed and this demonstrates that the simulation settings and temperature regulation procedures are not misleading. This concurrence with the concepts of basic statistical mechanics indicates that the simulated ensembles were kept in check throughout the trajectories (Allen et al., 2019).

The different profiles of potential energy distributions (Table 2, Figure 3) indicate the variations between the ordered and disordered states. Such differences aid in our knowledge of the changes that occur to the structure as a consequence of changing temperatures. The appearance of these differences can be considered in connection with alteration of the radial distribution functions (Table 3, Figure 4), according to which the peaks are also not so sharp at higher temperatures. This falls in line with the concept that atoms are less restricted it is less orderly. These types of tendencies have been discovered in many experimental and computational works focusing on liquids and amorphous solids (Tuckerman, 2020).

A more direct evidence that mobility is temperature dependent can be found in the mean-square displacement (MSD) and velocity autocorrelation function (VACF) analyses (Table 4-5, Figures 5-6). The increase of temperature leads to bigger values of the diffusion coefficients (Figure 7, Table 6) and decreases the decay of the VACF, that is, the momentum relaxation times will be shorter. This trend is consistent with what we know and what we would expect in thermally activated diffusion processes (Rapaport, 2018) and is consistent with experimental tracer diffusion data in similar systems.

The pressure and the energy stability test (Tables 78, Figures 89), reveal that the selected time steps of integration and ensemble controls maintained the thermodynamic equilibrium throughout the modelling. That the overall energy remains constant during microcanonical (NVE) testing implies that the number of numerical integration errors is minimal, which is highly desirable when conducting longer simulations (Frenkel & Smit, 2021). Such a degree of reliability is required in order to ensure that computations of dynamic properties (such as diffusion coefficients) are not influenced by artifacts of insufficient numerical stability.

As shown in Table 9 and Figure 10, structural order parameter analysis demonstrates that MD is quite handy in a period measurement of phase behavior. The findings illustrate how a greater amount of thermal energy disrupts the long scale order, which is pertinent in solid into liquid. As an illustration Figure 11 presents a hybrid display that interplays MSD and RDF data. This provides a fuller description of structural connections with dynamics that are needed in the explanation of the occurrence of phase transitions (Haile, 2019).

Overall, this paper indicates that MD simulations can reproduce known thermodynamic and transport processes well and can provide us minute details which are difficult to obtain with experimental techniques. Taken together, RDF, MSD, VACF, and thermodynamic property analysis comprise a powerful toolkit with which to determine just what is happening at the molecular level. The results also not only affirm that MD is a good method of making predictions but it also enables the application of the method in more complex systems such as biomolecular assemblies, nanomaterials and multicomponent fluids.

CONCLUSION

To sum it up, the discussion and results indicate the significance of molecular dynamics simulations in determining the behaviour of atoms and molecules. Such simulations have revealed the atomic structure, thermodynamic properties and dynamics of molecular systems to us showing us information new in many fields of science. Research with molecular dynamics is interdisciplinary, thus giving birth to new concepts. Such simulations are the significant aspects of scientific development and discoveries. Molecular dynamics simulations play a role in the exploration and new concepts as the scientists learn more about the nanoscale.

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