

# The Study of Simulating Metaloxide Nanoparticles In Aqueous Fluid.

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**Abstract**— Dynamics of nanoparticle dispersion in engineering fluids has a significant impact on the quality and performance of liquid based fluidic systems; such as in biomedical fluids, contaminated water system and its purifications. The dispersion dynamics of metaloxide nanoparticles in an aqueous fluidic system, was studied using large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) in this paper by using CuO particles as a targeting material in water (H<sub>2</sub>O) fluid system. Two major calculation parameters were selected for evaluating the system in the simulation: a) discrete particle dynamics (DPD), and b) smoothed particle hydrodynamics (SPH). Comparing experimental with the molecular dynamics (MD) simulation results shows good correlations with the MD viscosity as 1.44 mPas at 313K and diffusion coefficient of metaloxide nanoparticle-H<sub>2</sub>O system was obtained as  $1.03 \times 10^{-8} \text{m}^2/\text{s}$ .

**Keywords** --Nanoparticle dispersion in fluids • Molecular dynamics • Diffusion simulations • Copper oxide • LAMMPS

## I. INTRODUCTION

Nanoparticles provides large surface area to their volume ratio, which may reduce or enhance their diffusion capabilities in a fluidic system, and specifically controlling of this diffusion proved to be a challenging task [1, 2]. Several studies have focused on nano particle dispersion and stabilization in a base fluid such as water, to establish an effective methodology for a thorough dispersion of nano particles in fluidic systems [3-5]. The metal oxide nano particles (M O<sub>x</sub>) are the widely used in biomedical devices, environmental and water contamination research due to their environmental stability, functionality [6], thermo-mechanical [7-9] and physio-chemical properties [10, 11]. These types of nanoparticles including CuO, ZnO, MgO, CaO, and many others, are increasingly used in applications such as biomedical fluidic and water purification [12-14], as antibacterial additives and components and mostly the medical devices surface coating [6, 12, 15, 16]. Especially, in the water purification processes and biomedical applications, it is involving the releases of Cu<sup>2+</sup>, Zn<sup>2+</sup> and ionic particles that may result in disinfection of contaminations from bacteria pathogens [12-14]. As the metal oxide such as CuO nanoparticles (CuO-NPs) are common atomic structures and thermally and physically stable and cost-effective,

therefore, this study concentrated on investigating the CuO nanoparticle's dispersibility in water fluid system using molecular dynamics which is not yet reported [3, 4].

Simulations as a major prediction of the mechanism of nanoparticles dispersion in engineering liquids, is a fast and cost-effective alternative parallel to the experimental works. A number of diffusion simulations of polymeric, ionic and mineral nanoparticles have been extensively reported [17-19]. The major particle diffusion phenomena in these studies have been carried out is based on the Brownian dynamics (BD), targeting the random motion of the nanoparticle in a water fluidic system. One of the most accepted simulation parameters for the dispersion of metal oxide nanoparticles in a water system is the discrete particle dynamic (DPD) potential, which is used for assessing the power to disperse nanoclusters reflecting the phenomena of the Brownian dynamics [20, 21]. Studies using DPD for complex fluidic systems [22-24] shown that the dispersion of nanoparticles in water exhibits complex properties in simulation.

An initial selection of boundary conditions is carried out with a molecular dynamic simulator [25], working on cluster particle sizes, their force field interactions, diffusion in solvent, and physiochemical properties [26, 27]. Within the simulation system, force field is a mathematical parameter that governs the energies and potentials between interactive atoms controlled by the pair potentials between atoms. The physiochemical settings of the system referred to the thermal, chemical and physical properties of the system such as initial temperature settings, charges and dynamics of the system.

## 3 Materials

The CuO nanoparticles were prepared by thermal plasma forming technology (Tespia™) by QinetiQ Nanomaterial Ltd (Farnborough, UK). The bulk density of CuO-NPs is 6.3-6.49 g/cm<sup>3</sup>. The measurement of the CuO-NP average crystal size mixture is 22.6 nm.

The simulated CuO-NP configuration of crystal lattice was  $\alpha$  is 90°,  $\beta$  is 99.54° and  $\gamma$  is 90° with a space group of C2/c that was generated on a Material Studio software by Accelry Ltd.

## 4 Methodology

Experimental viscosity was measured in this work by using TA 1500Ex. The TA Instruments AR1500ex Rheometer is an advanced analyzer for measuring properties of rheology such as viscosity, shear rate, stress and strain. The experimental viscosity of CuO-water nanofluid system was measured to compare and support the MD results. The mixture of nanoparticles in the experiments were measured and calculated with a volumetric fraction of ~2% vol.

### 1.3 Simulation conditions: nanoparticles dispersed in water fluids

Metal oxide nanoparticles in water fluidic media were simulated by using COMPASS force field on condensed-phase optimized molecular Potential [26-29]. The COMPASS force field was used for computational energy calculations. This force field has been implemented for different molecular interactions from organics, inorganics, monomers, and polymers, to metals, metallic ions and metal oxides [26-29]. Green-Kubo formulation was also used shown in Equation 5 to extrapolate the system viscosity, which is a well-established method of computing the viscosity by autocorrelation functions equation 6. Later the results of the viscosity achieved through simulation are validated using stress autocorrelation function as shown in Fig.3.

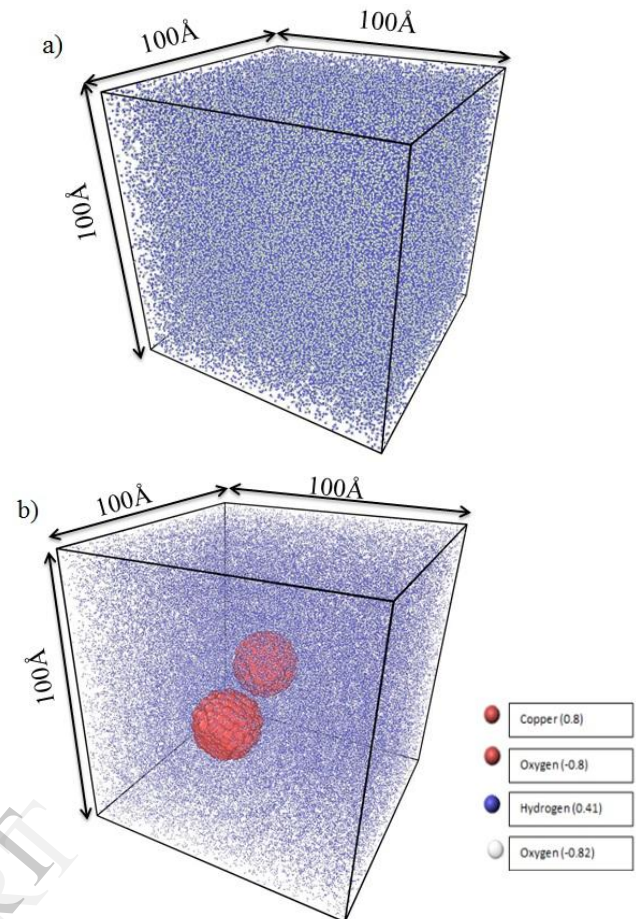
The Interactive parameters for the fluidic system used in this simulation are DPD and SPH potential for composing the diffusion model of the CuO-NP-water fluidic system. The DPD factor is explained by Equation 1, which composes of 3 force components, accounting for the particle random movement and momentum through the system.

$$\vec{f} = (F^C + F^D + F^R) \hat{r}_{ij} \quad (1)$$

These three forces (i.e.  $F^C$ ,  $F^D$  and  $F^R$ ) are comprised in DPD pair-style to execute the DPD action to perform the desired motion. The influence of the forces in particular directions is handled by  $\hat{r}_{ij}$ .

### 1.4 Simulation

The dispersing nanoparticles in water was simulated by using LAMMPS [30-32] composed of 80000 transferable intermolecular potential (TIP3P) water molecules [33]. The nanoparticles used in this study are in 80000 TIP3P water molecular system. The system was simulated with SPH and DPD potential in an imaginary orthogonal box (i.e., 100 Angstrom x 100 Angstrom x 100 Angstrom) shown in Fig.1. The initial simulation system was setup by using 3320 CuO molecules, which were represented by 2 nanoclusters each carrying 1660 molecules bonded by compass force field. Therefore, the simulated particles in this work are in the nanometre scale between 4-6 nm. This is due to the limitations of current lab-based computers, which are impractical for simulating particles larger than 10nm with particle volume fraction between 1.5-2% equivalent to the volume fraction used in the experiments. Simulation trajectories were visualized using OVITO the code free available by Alexander Stukowski [34].



**Fig.1** Molecular system comparison with and without CuO-NPs: a) simulation results (control) of pure water molecules in an Orthogonal box of 100 Angstrom x 100 Angstrom x 100 Angstrom, the box contained 80000 TIP3P water molecules, where white is oxygen and blue is hydrogen. b). Molecular system of 80000 TIP3P water molecules with 2 CuO-NPs of 4nm in an Orthogonal box of 100 Angstrom x 100 Angstrom x 100 Angstrom, where white is oxygen, blue is hydrogen and red is representing CuO-NP, under NPT (NPT ensemble enables the system to keep the pressure constant but the volume is varied) conditions i.e. 1 bar pressure at the temperature of 303K.

## 5 Results and Discussion

The simulations were carried out by resembling the nanoparticle simulation in the water fluidic system. Although the particulate did not reach the actual nanoscale size in the simulation, the results still proved valuable as it showed temperature effects on the system's viscosity and particle diffusion efficiency, which is mostly effected by the particle volume fraction [35]. The diffusion coefficient is a measure of the number of atoms movement with the change in position; it is dependent on the viscosity, size and shape of molecules. However, viscosity is a measure of resistance to the fluid flow and depends on the gradual deformation of shear stress. The equations used for calculating these variables, shown in Table 1 are the bases for analyzing and comparing the results with the experimental trends. The properties analysed using the MD simulation were dependent on the statistical mechanical calculation implemented by Green-Kubo. However, images shows a constant volume, whereas, during

the simulation due to implementation of NPT ensemble caused the volume of simulation box to vary. The variable definition and further statistical formula has been presented in Table

**Table 1** Diffusion coefficient and viscosity variables, definitions and the statistical mechanical formula, and their equations.

Property	Variable	Definition	Statistical Mechanical formula (Green-Kubo)
Diffusion Coefficient	$D$	$\dot{n} = -D \frac{\partial \phi}{\partial x}$ (2)	$D = \frac{1}{6} d \langle (r_i(t) - r_i(0))^2 \rangle / dt$ (4)
Viscosity	$\mu$	$F = \mu \frac{\partial U}{\partial x}$ (3)	$\mu = \frac{V}{3k_B T} \int_0^\infty \left\langle \sum_{x<y} P_{xy}(t) P_{xy}(0) \right\rangle dt$ (5)

Where  $\dot{n}$  is the diffusion flux,  $D$  is the diffusion coefficient and  $\frac{\partial \phi}{\partial x}$

is the concentration at a particular position as shown in equation 1;  $\mu$  (mPa·s) is viscosity for the system  $V$  is the

Brownian volume fraction ( $\text{\AA}^3$ ) of particles in the system,  $\frac{\partial U}{\partial x}$  Velocity in x direction,  $F$  is the magnitude of force in equation

3;  $r_i(t)$  radius of particle  $i$  at time  $t$  and  $r_i(0)$  radius of particle  $i$  at starting time in equation 4;  $T$  is the temperature (K) of the system and  $P_{xy}$  is the stress component for atoms (atm),  $t$  is time (ps),  $K_B$  Boltzmann constant in equation 5.

### Viscosity

The simulated viscosity of CuO-NP dispersed in water is coherent to the experimental values. The Green Kubo method utilizes stress tensor to analyse the viscosity. This stress tensor  $P_{xy}$  is the stress component between molecules of the x-y direction.

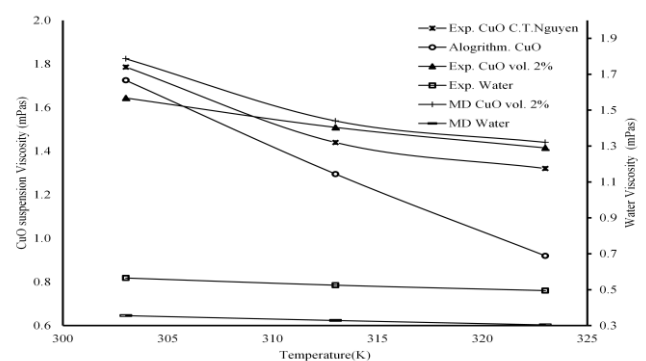
The viscosity from the TIP3P water model is decreasing with increasing temperature as shown in Figure 2. These simulation values are in good correlations with H.L. Tepper and Gonzalez results [36, 37], which were shown at temperatures around 298-300K giving the viscosity of TIP3P model as 0.321-0.311 mPas, whereas the experimental value obtained in this work was around 0.59 mPas. These values can further be compared with Min-yi Shen and Karl F. Freed's [38] achieved similar viscosity around 0.5 mPas at 300K using simulation technique of Langevin dynamics. The viscosity values obtained in this work were slightly higher due

1. Where  $n$  is the number of atoms,  $T$  is the temperature,  $t$  is time period,  $v_i$  is velocity of particle  $i$  and  $p$  is the shear stress in Table 1.

to the higher heat conduction through the system and dissipative particle dynamics potential.

A decrease was seen for the viscosity of the TIP3P water model with the increasing temperature of the system. This is a usual phenomenon for any liquid when temperature is increased while molecules started to expand which leads to anomalous decrease in viscosity shown in Figure 2.

High concurrent trend of experimental viscosity results [29] of dispersing CuO-NPs in deionized water were compared, with the algorithm-neural network (GANN) method [39], which are shown in Fig. 2 to the trend of molecular dynamic simulation results. Some studies relate that particle size shows negligible effect over the viscosity [40] while others suggest that a decrease in particle size gives a viscosity increase [41-44] and vice versa for other researchers [35, 45, 46]. The results of the system are averaged over the  $N$  number of particles in the system.



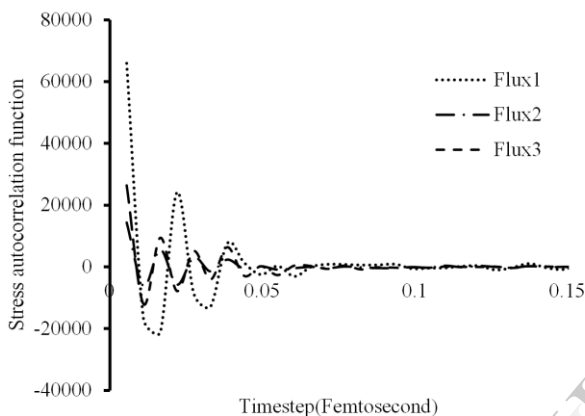
**Fig.2** Viscosity (mPa.s) comparison of the fluidic systems of experimental, MD simulation of CuO-water system, pure water, and the algorithm results [39] and experimental [35].

This size dependent system causes an increase in the number of runs and equilibration time. Later improvement of the statistical precision is achieved by three off diagonal element of the stress tensor.

### Stress Autocorrelation function (SACF)

The molecular dynamic viscosity was measured using the Green-Kubo method. This method uses an autocorrelation function to validate the results of viscosity. The viscosity validation is carried out using the stress autocorrelation function. This function uses three off-diagonal terms to analyse the system viscosity. These terms are  $P_{xy}$ ,  $P_{yz}$  and  $P_{xz}$  related to pressure fluctuations in different directions. The stress tensors in between the angular brackets as shown in equation 6 compute's averages of large number of samples. Where term  $P_{xy}$  computes the stress in x-y direction. The sample quantities consist of duration the MD simulation will run for,  $\Delta t$ , and N number of particles in the system.

$$C_{xy}(t) = \left\langle \sum_{x < y} P_{xy}(t) P_{xy}(0) \right\rangle \quad (6)$$



**Fig.3** Stress autocorrelation function graphs for validation of achieved viscosity of CuO NPs in water from MD simulation at 303k.

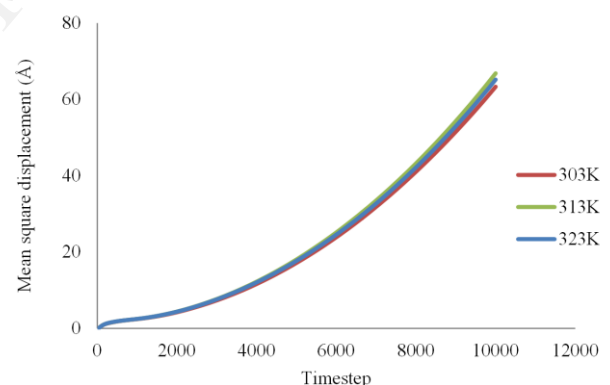
Further, the monotonic decay of the SACF relates to the successful achievement of rheological quantity i.e. viscosity in our case. The SACF took 0.07 fs to completely settle for 303k viscosity reading, whereas, for other two temperature readings of 313k and 323k took 0.07-0.09 fs.

### 1.5 Mean Square Displacement (MSD)

Diffusion coefficient was measured for analyzing the diffusion rate of the CuO in water using Equation 4, where  $D$  is diffusion coefficient ( $m^2/s^2$ ),  $r$  is the distance between consecutive particles and  $t$  is time (s).

The diffusion rate was calculated by the slope measurement of trend lines using one-sixth of the slope which gives the self-diffusion coefficient. The calculated MSD is shown in Fig. 4, by using the slope of these lines, the diffusion coefficient of CuO-NPs in water suspension at different temperatures of 303K, 313K and 323K was found. Table 2 lists particular diffusion coefficients of CuO-NP water suspension and pure water system. Later, Fig. 4 shows the CuO-NP water suspension MSD at different temperatures. The diffusion coefficient results obtained for this suspension model is similar with the result of CuO nano-rods diffusion coefficient in water by Cheong F.C et al. [47], they measured diffusion coefficient of CuO nano-rods with holographic video microscopy and obtained the value of  $2.31E-7 m^2 s^{-1}$  at 298K. However, there is a slight difference, this can be due to temperature and heat conduction through the system that causes the Brownian effect to change and consequently altering the diffusion.

In Figure 4 there is a linear increase in the diffusion coefficient ( $m^2/s$ ) of the water with temperature increase and this has been correlated by other studies of TIP3P water molecules [48]. This study investigated TIP3P water molecular diffusion coefficient at 320 K is  $2.272E10^{-9} m^2/s$ , which is in a good agreement with achieved value in this work as shown in table 2, together with other experimental value obtained from previous literature [49]. It is also known that by implementation of DPD helped in decreasing the computing time step for equilibrium convergence and higher accuracy [50].



**Fig.4** MSD of CuO nanoparticles in water suspension a) 303K, b) 313K, c) 323K.

**Table 2** Simulated diffusion coefficients of nanoCuO-water system and pure water system.

Temperature (K)	Diffusion Constant ( $m^2/s^2$ )	
	CuO-water system	Water system
303	$1.033 \times 10^{-8}$	$9.000 \times 10^{-9}$
313	$1.150 \times 10^{-8}$	$9.060 \times 10^{-9}$
323	$1.051 \times 10^{-8}$	$9.1066 \times 10^{-9}$

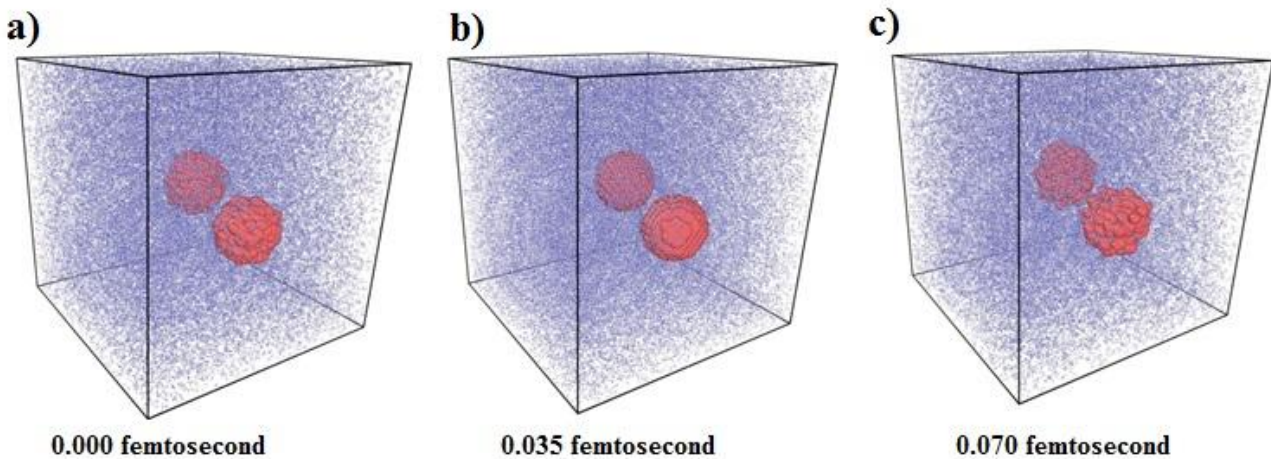


Fig.5 CuO-NPs water suspension system at 303K; 5a) 0.000 femtoseconds; 5b) 0.035 nanoseconds; and 5c) 0.070 femtoseconds.

Finally, the Fig.5 illustrates the simulation screen dumps of CuO water suspension at 303K. The Fig. 5a shows the screen dump at 0fs, the initial condition when simulation was just started, no atomic movement can be found. Later Fig. 5b demonstrates the simulation at an interval of 0.035fs. Here the simulation is approaching the equilibrium level of convergence as shown in Fig.3 of SACF. Further, Fig. 5c shows the simulation at final stage's or the time when the simulation has gained the equilibrium convergence. It can be seen in Fig. 5c that the nanoparticles structural shape has changed, this is due to the influence of hydrodynamic

boundary layer that forms around the nanoparticles while in a nanofluidic dispersion state. However, Brownian motion cannot be neglected here, since this influence on nanoparticles micro motions i.e. responsible for rotation and vibration of the particles in suspension.

The viscosity trends obtained through molecular dynamics simulation is in 4-6% contrast with experimental obtained values. The CuO-NPs simulated results of diffusion coefficient is found to be  $1.033 \times 10^{-8} \text{ m}^2/\text{s}$  at 303K, this can be correlated with the data found from literature [47].

## CONCLUSIONS

This study has demonstrated a simulative model prototype development, which can be used for different metal oxide nanoparticle's dispersion in aqueous fluid in terms of the viscosity and diffusion coefficients. Reproductions of self-diffusion constant of TIP3P water model in the system has been given to provide a comparative base for the system with CuO nanoparticles in diffusion interactions. However, concurrent trends and results have been achieved under the experimental and simulative conditions. It is investigated that the viscosity increment is dependent on

the volume fraction of particles rather than its size. It was seen that the molecular dynamic of 2% CuO nanoparticle suspension shows similar trend as 2% vol. of experimentally setup mechanism.

This study excavated the interactive dispersion mechanism of nanoparticles at molecular level in order to exploit the lab-based computer simulation capabilities towards the nanoparticles-water system in reflecting of some larger sized potential particles and multiple particle system for future considerations.

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**Abbreviation Table and their units**

Symbols	Meanings
CuO	Copper Oxide
CuO-NP/s	Copper Oxide Nanoparticle/s
H <sub>2</sub> O	Water
DPD	Discrete particle dynamics
MD	Molecular dynamics
BD	Brownian Dynamics
SPH	Smoothed Particle hydrodynamics
°K	Degree Kelvin (Temperature unit)
Å	Angstrom
mPa.s	Milli Pascal second (Viscosity unit)
m/s <sup>2</sup>	Meter per second square (Diffusion coefficient unit)
COMPASS	Condensed-phase Optimized Molecular Potential for Atomistic Simulation studies
$r_{ij}$	i-j atomic separation distance.
$\vec{f}$	Total force
F <sup>c</sup>	Conservative force linked to momentum
F <sup>D</sup>	Dissipative force
F <sup>R</sup>	Random force
$\hat{r}_{ij}$	Force in particular directions
$d_t$	Timestep size
$K_B$	Boltzmann constant
T	Temperature
t	Time period
F	Magnitude of Force
$\frac{\partial U}{\partial x}$	Velocity in x-direction
$\dot{n}$	Diffusion flux
D	Diffusion Coefficient
$\frac{\partial \phi}{\partial x}$	Molar concentration in x-direction
$r_i(t)$	radius of particle <i>i</i> at time <i>t</i>
$r_i(0)$	radius of particle <i>i</i> at starting time
$C_{xy}$	SACF Function
$P_{xy}$	Stress tensor in x-y direction
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
TIP3P	Transferable intermolecular potential 3P
TEM	Transmission Electron Microscope
$\mu$	Viscosity
$\alpha, \beta, \gamma$	Lattice parameters
MSD	Mean Square Displacement
SACF	Stress autocorrelation function