

IDENTIFICATION OF THE INTERACTION OF LITHIUM HEXAFLUOROPHOSPHATE SALT AND ETHYLENE CARBONATE (EC) SOLVENT IN LITHIUM ION BATTERY REDOX EVENTS USING CLASSICAL MOLECULAR DYNAMICS (MD) SIMULATION

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ABSTRACT

The aim of the research is to find the maximum velocity possessed by the molecules (Maxwell velocity distribution) of the solvation event of lithium hexafluorophosphate salt ($LiPF_6$) interacting with ethylene carbonate (EC) solvent. We examined the electrolyte simulation of the reaction between lithium ions (Li^+) and hexafluorophosphate (PF_6^-) with ethylene carbonate (EC) solvent while the potential involved is the Lennard Jones potential. We use the epsilon (ϵ) and sigma (σ) parameters of Lennard Jones. These parameters are the independent variables used as a reference in determining the response variable which is the velocity of the molecules. Due to the large number of molecules involving the parameters and response variables per molecule mentioned above, we use a microcanonical assembly system (N, V, E) where the number of particles (N), system volume (V) and energy (E) are constant. The energy kT and the distance between molecules σ of 1 are inputted to the program in order to facilitate the computer in the simulation process. Solvation events where lithium hexafluorophosphate ($LiPF_6$) salt and solvent ethylene carbonate ($(CH_2O)_2CO$) interact then in the final positions of particles (equilibrium) the result is almost symmetry randomly in all planes. The velocity used is the most frequent velocity (v_{mp}) and is related to the kinetic energy.

Keyword : Electrolyte; Maxwell velocity distribution; Lennard Jones potential

Introduction

In order to meet the demand for electricity in the future, batteries that can provide large electrical power, are lightweight, cheap and safe are needed. The revolution has led to the need for rechargeable batteries with large capacity but small size and weight.¹ Lithium batteries are one of the most successful battery technologies over the past 20 years.² Regular rechargeable batteries have limitations in energy density and large size and weight. Commercial lithium ion batteries generally use lithium hexafluorophosphate ($LiPF_6$) in organic solvents as an electrolyte because it has high ion conductivity. The organic solvent propylene carbonate (PC) has an advantage over other organic carbonate

solvents because of its low price and good performance at low temperatures.³ However, the use of PC in lithium ion batteries has problems due to the cointercalation of solvent molecules with Li^+ ions on graphite and causing flaking. Organic solvents such as ethylene carbonate (EC) can form a solid electrolyte interface layer that is more stable than other organic solvents.⁴

Lithium batteries are capturing the portable electronics market due to their long cycle life. The commonly used anode is graphite with a lithium metal oxide cathode. The commonly used electrolyte is lithium salt in an organic solvent such as ethylene carbonate.² A lithium-ion battery consists of a graphite anode (negative electrode), a Li oxide cathode (positive electrode), and an

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ethylene carbonate (EC) electrolyte solution containing Li^+ ions and negative counter ions (usually PF_6^-). Diego et al performed MD simulations with the LAMMPS program where thermal degradation of the electrolyte appears. Experiments have been conducted to investigate the degradation of electrolytes, and it was found that DMC, EC, and DEC mainly contribute to gaseous products during thermal degradation, while DMC is relatively stable. Thermal degradation of electrolytes can produce PF_5 , CO_2 , ether, and alkyl fluoride. The detailed thermal degradation process is still unclear. It is difficult to experimentally capture the complex thermal degradation process and its intrinsic mechanism. Molecular simulation can provide significant insights.⁵ MD simulation has also been used by other researchers to reveal electrolyte characteristics. Effect of ($LiPF_6$) salt concentration on ionic diffusivity and conductivity, demonstrating maximum conductivity at a salt concentration of 1 M.⁶ Kumar examined the behavior of ($LiPF_6$) in EC solvent, using MD and DFT, focusing on solvent structure with Li^+ and PF_6^- ions. ion solvation and diffusion with ab initio MD simulations, showing that Li^+ ions can dissolve.⁷ The diffusion coefficient of Li^+ ion in EMC is proven to be greater than in EC, and the diffusion coefficient of PF_6^- is higher than that of Li^+ ion. This applies to regular and non-degraded electrolytes suggested by MD simulations. Studied the degradation mechanism of electrolytes and its impact using molecular simulations.⁸

Given the background above, the researcher conducted a study entitled "Identification of Interactions between Lithium Hexafluorophosphate Salt and Ethylene Carbonate Solvent in Lithium Ion Battery Redox Events Using Classical Molecular Dynamics (MD) Simulation". The simulation to be examined is the reaction between Li^+ ion and PF_6^- ion with EC solvent using the Lennard Jones 12-6 potential. Eventual solvation occurs when $LiPF_6$ salt and solvent $(CH_2O)_2CO$ interact, and the results can be observed in the

coding's final positions of particles (equilibrium event). The results should be symmetrical randomly in all planes. Researchers use Lennard-Jones parameters epsilon (ϵ) and sigma (σ) and the statistical mechanics system used is the microcanonical ensemble.⁹ The independent variable that is a key parameter in this research is speed, and from the speed of the molecules, the energy of the system can be determined. The aim of the study is to find the Maxwell velocity distribution. Each molecule has varying energy, but its appearance will be more accurately seen if we observe the speed distribution, while speed itself is related to kinetic energy. When lithium hexafluorophosphate ($LiPF_6$) interacts with the solvent ethylene carbonate (EC), a solvation event occurs and this causes molecules to move randomly as seen in the classical MD simulation Figures 5, 6, and 7. The coding performed by the researchers utilized the Verlet algorithm, which allowed for the determination of the final positions of particles after equilibrium was achieved. Based on articles that have been created by Hossain et al (2020), Iizuka et al (2021), Kumar et al (2016), Diego et al (2017, 2019), Ravikumar et al (2018), Tianhan et al (2019) This research has never been done by other researchers. This study uses Classical Molecular Dynamics (MD) Simulation which aims to Identify the Interaction of Lithium Hexafluorophosphate Salt and Ethylene Carbonate (EC) Solvent at the time of salt and solvent solvation events, solvation will take place when the battery redox reaction takes place. The microcanonical assembly system (N, V, E) has also never been used by other researchers on the interaction of the EC salt and solvent.

Methods

Although the method in this research is a model or simulation using classical MD in finding the probability of Maxwell velocity distribution, theoretical studies and literature studies based on research (research works) that have been published by other researchers are also carried out as foundation data to

build this simulation. The computer as a tool and software used is Scilab. Soetens et al used a combination of 12-6 Lennard Jones parameters from the OPLS AA force field.¹⁰ Molecular dynamics simulations performed for *Li* dissolved in ethylene carbonate (EC), propylene carbonate, and dimethyl carbonate revealed that lithium ions are dissolved by the electrolyte in tetrahedral coordination.¹⁰ The same unbound interaction parameters along with modified AMBER.¹¹ parameters for bound interactions were then used.¹² to study the structure and vibrational properties of lithium ions dissolved by EC.¹² The solubility of several lithium salts in EC and dimethyl carbonate was studied using a simulation package using COMPASS force fields with ESP charges obtained with PBE functionals.¹³ The van der Waal parameters were obtained directly from Accelrys automatic parameter generator (Material Studio). The unbound interaction parameters along with the charge for EC were taken from Masia et al.¹² while the *PF6* parameters were taken from Jorn.¹⁴ except the Lennard-Jones parameter sigma for phosphorus which was taken from the universal force field (UFF).¹⁵

This study used the Lennard Jones potential 12-6¹⁶ the parameters of which are listed in Table 1^{12,11,14,15}. Harmonic force bond stretching ($Kb = 370.8 \text{ kcal/mol}$ and $bo = 1.606 \text{ \AA}$) and angular bending ($K\theta = 139.4$ and $\theta^0 = 90^\circ$) were used for PF anions.¹⁷ The dynamic properties of lithium ions in electrolyte solution were characterized in terms of diffusion coefficient as well as ionic mobility.

Simulations were performed where the particles in the box satisfy Newtonian mechanics and interact through the Lennard Jones potential. The researcher took the system with fixed number of particles, fixed volume and fixed total energy (N,V,E).⁹ The set of particles in the box size l_x , l_y and l_z . First, the initial conditions must be set, each particle can be informed to be equally distributed or can be randomly placed as long as the particles do not overlap each other. We give an appropriate initial velocity to all

particles. The equation of motion of an individual particle is in pers (1) Atom i experiences a force (Newton's equation), the force experienced by atom i is equal to the mass of atom i multiplied by the acceleration. The force is related to the potential energy of the system, where the force is the derivative of the potential energy with respect to the coordinates of the i -th atom. The force in a conservative system is the potential energy gradient. Integrate the equation for all particles and calculate.

$$m \frac{d^2 r_i}{dt^2} = F_i = -\nabla V \tag{1}$$

New position and velocity, using the velocity-verlet algorithm. Having to continuously update the position and velocity with time, once equilibrium is reached, we can evaluate the number of relevant statistics.

An overview of the algorithm in the form of a flowchart is shown in Figure 1, where the initial parameters or parameter constants have not been set then initialize the position (x, y, z) and velocity (v_x, v_y, v_z) of the particles. For this initialization, the initial total force must be calculated and then update the position of all particles, say the old force and calculate the new force on all particles. Update the velocity using the old and new forces, again we have to update the positions of all the particles. We have to keep repeating these three steps until equilibrium is reached (dotted line in Figure 1).

Table 1. Non-bonded LJ parameters used for simulation of *LiPF₆* dissolved in EC. O_x and C_x are carbonyl oxygen and carbon respectively, O_s is ether oxygen, C is carbon in hydrocarbon EC

Atom/pair types ^a	ϵ (kcal/mol)	σ (Å)
O_x	0.210	2.96
C_x	0.105	3.75
$Li - O$	0.20937	2.0217
C	0.066	3.50
H	0.030	2.50
Li	0.20314	1.4424

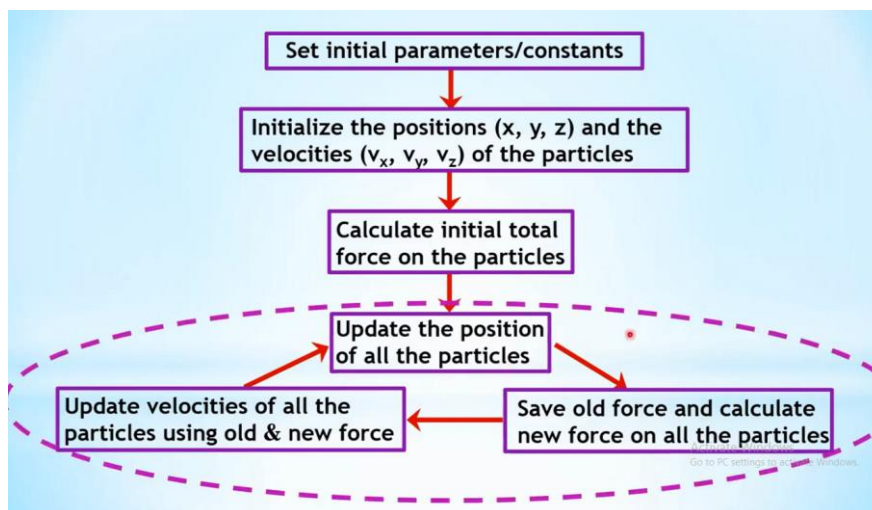


Figure 1. The algorithm is in the form of a flowchart, where the initial parameters or constant parameters have not been set then the initialization of the position and velocity of the particle is carried out.

```

sig=1;ep=1;m=1;lx=20;ly=lx;lz=lx;np=512;ni=2000;dt=0.005;va=3.4641016;
rc=2.5;avx=0;avy=0;avz=0;t2=0.0000125;t1=0.0025;
fc=-0.0389995;Vc=-0.0163169;
  
```

Figure 2. Initial coding for writing constants which the researcher summarized so as not to complicate computer work

```

// Main Program
[x,y,z]=posinit(); //position intialization
x1=x;y1=y;z1=z;
[vx,vy,vz]=velinit();
[fx,fy,fz,PEN]=forcecalc(x,y,z); //initial force calculation

for k=1:ni
[x,y,z]=updatepos(x,y,z,vx,vy,vz,fx,fy,fz); //update position
fox=fx;foy=fy;foz=fz; //save old force
[fx,fy,fz,PEN]=forcecalc(x,y,z); //update force
[vx,vy,vz,KEN]=updatevel(vx,vy,vz,fx,fy,fz,fox,foy,foz);
PE(k)=PEN/np; //average PE per particle
KE(k)=KEN/np; //average KE per particle
nit(k)=k; //no. of steps or iterations
disp('Iterations: '+string(k));
end
  
```

Figure 3. The main program provides functions for computing the initial position and velocity as well as updating the position and velocity during data processing.

The potential depth is ϵ and σ is the minimum distance that two particles can approach. Figure 2 illustrates the initial coding for writing constants which the researcher summarizes so as not to complicate computer work. Actually in Figure 2 this coding is specifically for sig and ep taken in Table 1, intentionally simplified here by using the value 1 because it represents about 6 calculation data (see

Table 1). As an example for 1 calculation data is for O_x oxygen carbonyl which has a value of $\epsilon = 0.210$ and $\sigma = 2.96$. In Figure 3, the main program is presented where there are subprograms that provide functions for computing the initial position and velocity as well as updating the position and velocity during data processing (not presented here). For the number of iterations (np) here, we used 100 and 1000 iterations in order to be

accurate to the Maxwell velocity distribution data. The length of the cube box (lx) is 20 and the number of particles (np) is 512. Along with that length, the box lengths (ly) and (lz) are also equal to (lx). Kinetic energy and potential energy are also presented here

```
for i=1:np
velocity(i)=sqrt((vx(i))^2+(vy(i))^2+(vz(i))^2);
end

//Plot Maxwell speed distribution curve
subplot(2,2,4)
histplot(20,velocity,polygon=%t);
xlabel('Speed of the particles','fontsize',6);
```

Figure 4. The velocity in this coding is the particle velocity in three directions: x, y and z axes. The histplot function will describe this simulation in detail

Which molecules are more dominant at room temperature. The independent variable that is the key quantity in most of these studies is the velocity of the molecules. From the velocity of the molecules, the energy of the system can be determined. Indeed, in the system (N, V, E), the energy is constant, but after a chemical reaction (in this case a simulation), the speed between the molecules will experience random movements, which in fact we can calculate the speed based on this simulation. The coding building is in Figure 4, where velocity is the particle velocity in 3 directions, namely the x , y and z axes. The histplot function will describe this simulation in detail. Sigma σ in the coding is written with sig which is the minimum distance that can be approached by 2 particles in units of Å. The mass m between two molecules is the reduced mass made to be 1 to facilitate computation in the simulation process but to calculate the initial time, the reduced mass of the molecules is still included. At 300 K, the energy kT of $4,14 \cdot 10^{-21} J$, again not calculated in this study in order to facilitate the computer in the simulation process. The initial time when the molecule is in the initial position state is given as follows in press (2):

$$t = \sqrt{\frac{ml^2}{E}} \quad (2)$$

where keep in mind here that researchers use space in the microcanonical assemblies system (N, V, E), where the number of particles N , volume V and energy E are fixed. Deliberately made fixed so that researchers can find out the interaction

Where t can be calculated by entering the dimensions of the reduced mass m in units of kg , the distance between 2 atoms l in units of m and the molecular energy E in units of J , the time can be $\sim 10^{-12} s$.

Result and Discussion

Researchers made MD simulations using scilab 6.11 software and obtained the results as shown in the figures below. The data for ϵ and σ are taken from Table 1. Figure 5 for carbonyl oxygen O_x calculation data $\epsilon = 0.210$ and $\sigma = 2.96$, where the iteration used by researchers is 100 iterations. Why the interaction chosen is only between oxygen and carbon atoms, this is because in solvation events where redox events occur, oxygen and carbon atoms perform non-bonding bonds and we know that oxygen and carbon atoms are owned by the EC solvent, as if it is only EC that plays a role, this is not the case, some molecules in EC are bonded, therefore it is not relevant to use the Lennard Jones potential. Not only do non-bonding interactions apply to the solvent, all molecules of the $LiPF_6$ salt also perform Lennard Jones interactions with the EC solvent as shown in Figure 8. We only simulated the data listed in Table 1 where epsilon (ϵ) and sigma (σ). Epsilon is the binding energy between atoms and sigma is

the distance between atoms, researchers chose lithium and oxygen bonds only. The reason for this selection is because researchers see that the most probable speed has almost the same value on the other hand if all interactions are included, the computer will be overwhelmed when iterating.

Figure 7 for the calculation data of C_x carbonyl oxygen $\epsilon = 0.105$ and $\sigma = 3.75$ with 1000 iterations. Figure 8 for Li-O calculation data $\epsilon = 0,20937$ and $\sigma = 2,0217$ where the iterations are 100. For Figure 5 where the iterations are 100, the distribution velocity of the Maxwell's value is 1.9

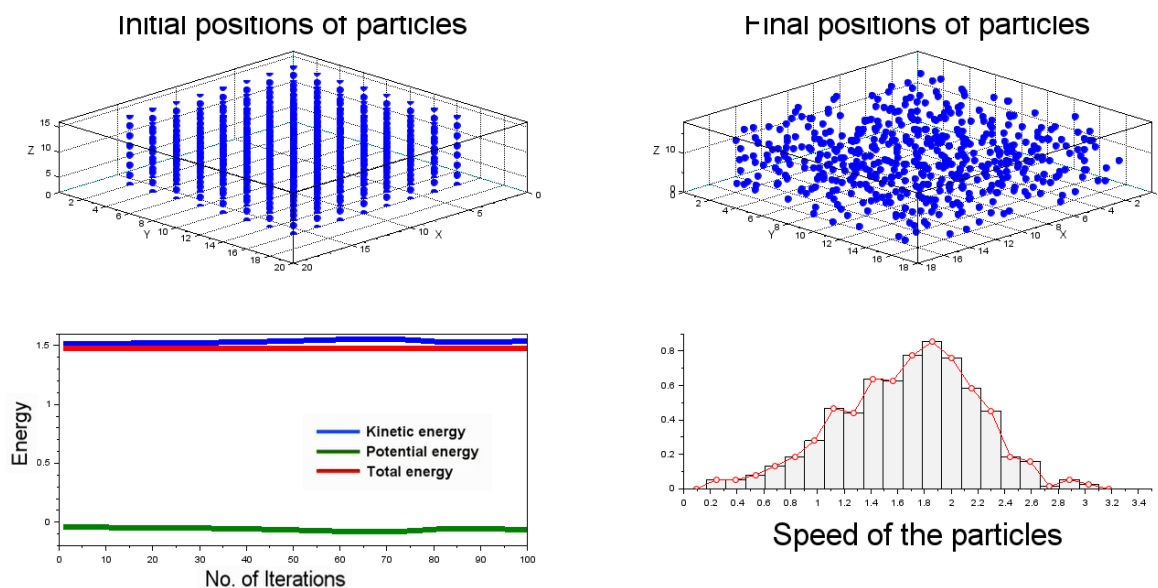


Figure 5. O_x calculation data of carbonyl oxygen $\epsilon = 0.210$ and $\sigma = 2.96$, where the iteration used by researchers is 100 iterations In salt solvation events Oxygen from the solvent EC

For Figure 7 for the C_x (carbon oxygen) interaction where the iteration is 1000, the Maxwell distribution speed is 1.7. The curve is not regularly distributed either, the same thing as before, namely the selection of the number of iterations that is not so appropriate, the number of iterations should be increased to 3000 iterations. At room temperature, 300 K, the kT energy of 1 is inputted to the program in order to facilitate the computer in the simulation process. The initial time when the molecule is in the initial position state is given in press 2. Where t can be calculated by entering the dimensions of the reduced mass m which is in units of kg , the distance between 2 atoms l in units of m and the molecular energy E in units of J then the time can be of order $\sim 10^{-12} s$. The distance between 2 atoms is 1 worth 1 \AA or if converted in SI MKS units to $10^{-10} m$. The

value of $l = 1 \text{ \AA}$ is because the coding has entered the value of σ for each molecule, it will indeed make it more difficult for the computer to calculate if the value of σ is entered first but the researcher entered this value because the iteration chosen was not up to 4000 iterations. If the iterations amounted to 4000 then the researcher had to replace the value of σ to be worth $\sigma = 1 \text{ \AA}$. Table 2, provides useful information in this regard. When lithium hexafluorophosphate ($LiPF_6$) salt interacts with ethylene carbonate (EC) solvent, the cation Li^+ becomes bound to the anion PF_6^- and surrounded by EC solvent. The ion pair consists of cations and anions that are in close contact in solution, rather than being separated by the solvent which can be seen in Figure 6. The ions in the ion pair are held together by the same electrostatic force in the

ionic solid. The Li^+ and PF_6^- ions in pair form migrate as a unit. If it is in the form of an ionic solid, the cation-anion interaction can be restrained in a rigid arrangement while

if it is in a completely dissociated ion solution, the cations and anions are completely surrounded by solvent molecules and are free to migrate.

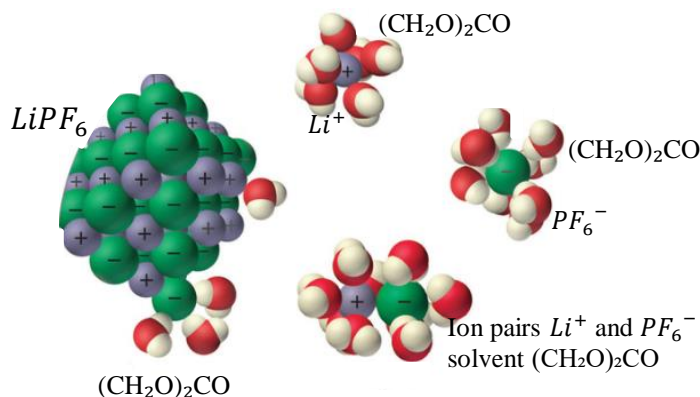


Figure 6. The Li^+ and PF_6^- ions in the form of a pair migrate as a unit, in the perfectly dissociated ion solution, the cations and anions are completely surrounded by solvent molecules and are free to migrate

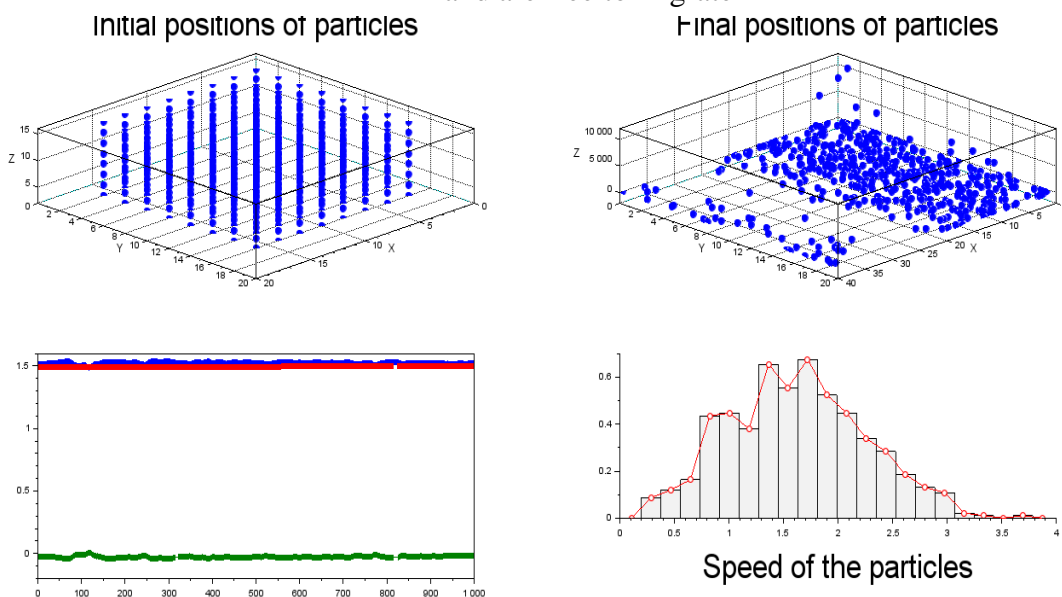


Figure 7. C_x calculation data of carbon oxygen $\epsilon = 0.105$ and $\sigma = 3.75$ with 1000 iterations

In Figure 5 specifically for interaction 100, the reaction response is in a solvation event where the $LiPF_6$ salt and the solvent ethylene carbonate $(CH_2O)_2CO$ interact. The molecular ion pairs Li^+ and PF_6^- as well as the solvent $(CH_2O)_2CO$ in the form of blue spheres (for more details in Figure 6). Since the number of iterations is only one hundred, in the final positions of particles the result is a random motion that is almost symmetrical

in all planes (x, y and z). This final position indicates that the system has reached equilibrium.

The above microcanonical assemblies can be connected to the canonical assemblies of the system (N,V,T) by using the ensemble as a virtual space to record a large number of microcanonical assemblies⁹. The purpose of this recording is to obtain Thermodynamic quantities namely energy, enthalpy,

Helmholtz energy and the most relevant from battery research is Gibbs energy. The virtual recording can be connected to the real world by using probabilities and in the probabilities there is a partition function on the ensemble. Once again microcanonical assemblies, canonical assemblies and canonical ensembles are the three ways to solve problems in the microworld. Although this microcanonical assemblies system seems simple, the coding made by this researcher will be very helpful in finding the average energy in this assemblies system. Each molecule has a variety of energies as shown in the simulation of Figures 5, 7 and 8, but its appearance will be seen more accurately if we look at Maxwell's velocity distribution in these figures and Table 5. This microcanonical assemblies system can help ab initio molecular dynamics simulations. Particularly in this study, the use of coding in the microcanonical assemblies system that represents an isolated system that has a fixed energy. Ab initio molecular dynamics (AIMD) is a powerful tool to predict the properties of molecular systems. AIMD simulations sample the potential energy surface of a system at constant energy (microcanonical) and at constant temperature (canonical).

At the time of the initial positions of particles (see Figure 5), it is assumed that no redox event has occurred, there is no external force field from outside that serves to move the molecules. External force fields can exist in charge and or discharge events. The most frequently occurring velocity (v_{mp}) for oxygen carbonyl (O_x) is 1132 m/s then its kinetic energy is $1,1 \cdot 10^{-21} \text{ J}$. The most frequently occurring velocity (v_{mp}) for carbon oxygen (C_x) is 1013 m/s then its kinetic energy is $8,72 \cdot 10^{-22} \text{ J}$. The most frequent velocity (v_{mp}) for ether oxygen (O_s) is 1407 m/s , the kinetic energy is $2,82 \cdot 10^{-21} \text{ J}$. The kinetic energy is the internal energy of carbonyl oxygen (O_x), carbon oxygen (C_x) and ether oxygen (O_s). The question is whether these interactions are discrete interactions, the answer is not at all. When lithium hexafluorophosphate salt

($LiPF_6$) interacts with ethylene carbonate (EC) solvent, a solvation event occurs and we already know that in non-bonding bonds, the potential at play is the Lennard Jones potential. The interaction simulation of carbonyl oxygen (O_x), carbon oxygen (C_x) and ether oxygen (O_s) carried out in this study is a microcanonical assemblies which refers to an isolated system whose energy is constant (N,V,E). The system is considered isolated and cannot exchange energy or particles with the environment. Figures 5, 7 and 8, have not included the temperature value while the calculations in Table 5, researchers have entered the temperature value of 300 K (room temperature). Visualization of the scattering of molecules in the system (N,V,E) will look like in Figures 5, 7 and 8. Initial positions of particles show the initial state of the particles, it should be emphasized here that the initial state here is an idealized state where in the initial position the particles will be located symmetrically dividing the entire 3-dimensional space. Coding using the Verlet Algorithm, the final positions of the particles after equilibrium can be determined.

In Figure 7, for carbon-oxygen C_x calculation data $\epsilon = 0.105$ and $\sigma = 3.75$ with 1000 iterations, in the Brownian motion pattern the molecules gather in a plane where equilibrium has not been reached. We know that there should be no empty space in this case because nature abhors a void therefore the visualization with 1000 iterations does not meet the conditions of the real situation. In a short situation in the order of picoseconds (ps), this may happen but the next time the molecules will take the same position again in all planes. In Figure 8 the iterations are only 100, intentionally the researcher did that because specifically for visualization, the molecules will take the same part in all planes. The last estuary of this research is to determine the Gibbs energy of the system this cannot be done yet because more information is needed in particular. Indeed, Gibbs energy can be found by using a microcanonical assemblies system but it cannot be brought into the real world because

the system is an isolated system with constant energy. Systems that are closer to the real world are canonical and grand canonical assemblies. Canonical assemblies are more popular because the battery (system) will interact with the environment where its energy will undergo changes. Actually, it is not the battery as a system but here more specifically, the system is lithium hexafluorophosphate salt and ethylene

carbonate $(CH_2O)_2CO$. The next hope is to create coding for canonical assemblies of (N, V, T) and (N, P, T) simulations. The Gibbs free energy of the reactants can be used to determine the maximum amount of work the battery can do. The reactants are lithium hexafluorophosphate salt and ethylene carbonate $(CH_2O)_2CO$. Gibbs free energy and cell voltage are directly related.

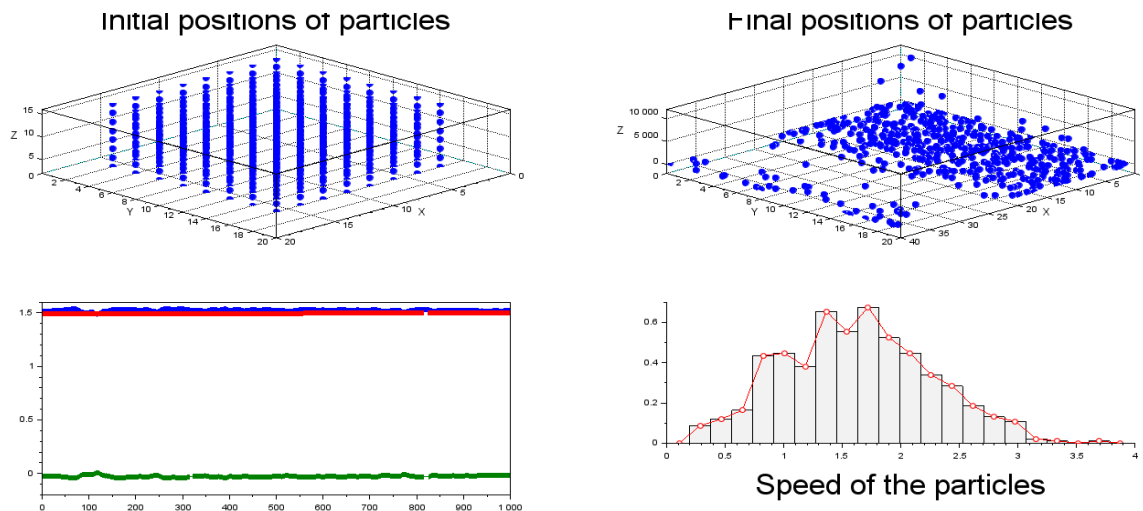


Figure 7. C_x calculation data of carbon oxygen $\epsilon = 0.105$ and $\sigma = 3.75$ with 1000 iterations

Table 2. The initial time of press (2), t is calculated, the distance between 2 atoms l and the molecular energy E in units of J.

	Reduction mass (kg)	Inter-atomic distance l (m)	Start time t (sec)	valu e	v_{mp} (m/s)	v_{mp} theoretical I (m/s)	v_{avg} theoretical (m/s)
Carbon oxygen (O_x)	$1,17 \cdot 10^{-26}$	$1 \cdot 10^{-10}$	$5 \cdot 10^{-13}$	1,9	1132	843	951
Carbon oxygen (C_x)	$1,17 \cdot 10^{-26}$	$1 \cdot 10^{-10}$	$6,3 \cdot 10^{-13}$	1,7	1013	843	951
Oxygen ether (O_s)	$4,18 \cdot 10^{-27}$	$1 \cdot 10^{-10}$	$3 \cdot 10^{-13}$	1,83	1821	1407	1588

Conclusion

The independent variable that is the key quantity in most of these studies is the velocity of the molecules. Researchers have made MD simulations and obtained the

results shown. The number of iterations is not very precise. The energy kT and the intermolecular distance σ of 1 were input to the program in order to facilitate the computer in the simulation process. Cations and anions are completely surrounded by

solvent molecules and are free to migrate. Solvation events where the $LiPF_6$ salt and the solvent $(CH_2O)_2CO$ interact then in the final positions of particles (equilibrium) the result is almost symmetry randomly in all planes. The coding that this researcher has made will be very helpful in finding the average energy. Each molecule has a variety of energies but their occurrence will be seen more accurately if we look at the velocity distribution, while velocity in itself has a relationship with kinetic energy. When the lithium hexafluorophosphate salt ($LiPF_6$) interacts with the ethylene carbonate (EC) solvent, a solvation event occurs and this event will cause random molecules as shown in the classical MD simulation Figures 5, 7 and 8. The coding that researchers do is using the Verlet Algorithm, and the final positions of the particles after equilibrium can be determined.

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