

Monte Carlo Simulation to Determine the Average Energy of Lithium Hexafluorophosphate, Ethylene Carbonate, and Vinylene Carbonate Electrolytes

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ABSTRACT

This study aimed to determine the average Lennard-Jones (LJ) potential energy of a lithium hexafluorophosphate (LiPF_6), ethylene carbonate (EC), and vinylene carbonate (VC) system using Metropolis Monte Carlo (MC) simulation at 300 K. The first simulation used 200 particles, a box length of 60 Å, and 10000 steps, giving a running average energy of 5240.59 kJ/mol, and the system had not reached equilibrium. Extending the same system to 100000 steps gave 522.77 kJ/mol. The third simulation used 400 particles (100 of each species), $L = 200$ Å, and 10000 steps, giving 0.25 kJ/mol, again without convergence. The fourth simulation used 400 particles, $L = 200$ Å, and 100000 steps, giving -0.53 kJ/mol, which indicates net attractive interactions under the employed LJ parameters. The running average of this simulation converged. The large decrease in energy mainly reflects the lower particle density in the larger box. Convergence of the running average does not by itself validate the energy value, and no activation energy was determined.

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1. INTRODUCTION

The development of better electrolytes for lithium-ion batteries has become increasingly urgent because lithium hexafluorophosphate-based batteries are currently widely used but still have limitations in terms of safety, performance, and lifespan. LiPF_6 is known to be unstable at high temperatures and easily decomposes, producing HF and PF_5 , which can trigger exothermic chain reactions leading to thermal runaway. Therefore, understanding its behavior under various temperature conditions is essential for the development of safer batteries (Mynam et al., 2021). A lack of understanding of the thermal degradation mechanisms and their effects on electrolytes also hinders improvements in battery performance and lifespan (Gao & Lu, 2019; Spotte-Smith et al., 2022; Xu et al., 2024). On the other hand, the solid electrolyte interphase (SEI) layer formed on the anode plays a crucial role in determining battery lifespan; however, its formation process occurs on time and spatial scales that are difficult to observe experimentally. The multiscale model developed by Yu et al. (2023) demonstrates that combining electrochemical models with Monte Carlo (MC) simulation can effectively analyze the effects of various parameters on battery performance with good accuracy. Meanwhile, molecular dynamics (MD) simulations conducted on silicon anodes help in understanding the charging process and serve as a reference for the development of improved batteries (Gálvez-Aranda et al., 2017). MC

and Kinetic Monte Carlo (KMC) simulations play an important role in bridging reaction mechanisms at the atomistic scale with SEI formation at the mesoscale (Wagner-Henke et al., 2025), enabling the modeling of vinylene carbonate (VC) polymerization and SEI formation up to the millisecond timescale. This approach allows for the virtual exploration of electrolyte compositions incorporating additives such as VC into mixtures of LiPF_6 and ethylene carbonate (EC) before physical testing is carried out, thereby reducing the time, cost, and risks associated with experiments (Gavilán-Arriazu et al., 2021). Thus, this research not only contributes to the fundamental understanding of electrochemical processes at the molecular level but is also essential for supporting the development of safer, more efficient, and longer-lasting batteries to meet the demands of the global energy transition (Perez-Beltran et al., 2024; Zelič et al., 2025).

Previous studies have shown that LiPF_6 , as a standard electrolyte salt, can improve the performance and stability of lithium-ion batteries; however, its behavior is highly temperature-dependent and therefore requires further investigation to ensure battery safety and reliability. The mechanisms of thermal degradation in electrolytes are also known to affect battery performance and lifespan, and these effects have been examined in several previous studies (Gao & Lu, 2019; Spotte-Smith et al., 2022; Xu et al., 2024). Previous modeling studies have developed multiscale models that integrate electrochemical models with MC simulations to analyze SEI layer growth and the effects of various parameters on battery performance. In addition, MD simulations have been employed to understand the charging process in silicon anodes as an alternative to graphite. In general, MC and MD simulations have been proven capable of modeling lithium-ion solvation structures, ion transport properties, and predicting battery performance across micro-to-mesoscale systems (Tian et al., 2023). MC-based and related computational approaches have been applied to model lithium-graphite intercalation compounds (Anniés et al., 2021) and to analyze cell-to-cell variability (Barbers et al., 2024). Regarding KMC simulations, the literature indicates that this method has been used since 1994 to study Li^+ transport, interfacial phenomena, and SEI formation, while also being capable of bridging *ab initio* reaction mechanisms with structures evolving over longer timescales (Gavilán-Arriazu et al., 2021; Wagner-Henke et al., 2025). Average energy has also been recognized as an important parameter related to activation energy and reaction rates in KMC models (Ntioudis et al., 2023).

An unresolved research gap remains in that although many three-dimensional KMC models have been developed to simulate the initial formation of SEI on lithium metal surfaces, these models have only been applied to highly simplified electrolyte systems and have not yet considered the effects of electrolyte additives (Wagner-Henke et al., 2025). Wagner-Henke et al. (2025) also states that although average energy is related to energy barriers and activation energy, this relationship has not been explicitly addressed in previous research. Therefore, the present study attempts to fill this gap by incorporating vinylene carbonate additives into a mixture of LiPF_6 and ethylene carbonate, as well as determining the average energy of the reactants to support KMC simulations in predicting reaction rates and SEI formation in more complex and realistic electrolyte systems. The approach employed in this study involves Markov Chain MC simulations to calculate the average energy of the reactants, which is intended to be used as input for future Kinetic Monte Carlo (KMC) simulations to model SEI formation in the $\text{LiPF}_6 + \text{EC} + \text{VC}$ electrolyte system. First, the Markov Chain MC simulation was performed to generate system configurations consistent with the Boltzmann distribution. From this stationary configuration, the average potential energy of the system was calculated, representing the internal energy within the canonical ensemble. The average energy is not an activation energy; it is intended only as a baseline quantity for estimating activation energies in future work. In a subsequent KMC study, the activation energies would be used to determine the reaction rates and transition probabilities of each event on the mesoscale time domain. Through this approach, the results may serve as a baseline for future KMC studies of SEI formation and VC polymerization over millisecond timescales, which are difficult to reach using conventional molecular simulations. In addition, the modeled system includes VC additive, which is known to influence the structure and stability of the SEI.

The combined MC–KMC strategy has been proposed as a way to reach timescales beyond those of MD, to include additives such as VC, and to move from equilibrium thermodynamic properties to reaction kinetics (Galvez-Aranda et al., 2017; Yu et al., 2023; Wagner-Henke et al., 2025). In the present

work, only the first step, a Metropolis MC calculation of the average potential energy, is performed. The KMC stage is left for future work.

The next section of this paper discusses the results and analysis of the simulations that were performed, particularly regarding the calculation of the average energy in the LiPF_6 , ethylene carbonate, and Vinylene Carbonate electrolyte system using the Markov Chain MC method. Four Metropolis MC simulations were performed, varying the number of particles, box length, and number of steps. Convergence of the running average energy was assessed with the cumulative average method defined in the Method section. KMC simulations were not performed because activation energies have not yet been determined; the average energies reported here are baseline values for future work.

The results and conclusions presented in this study concern the average energy values rather than the activation energies. Determining the activation energies requires further analysis using advanced approaches, such as the Arrhenius equation, Transition State Theory (TST), the Nudged Elastic Band (NEB) method, Umbrella Sampling, or fitting diffusion data obtained from MD simulations. The average energy is not equivalent to an activation energy. Thus, the average energy obtained in this study can serve as a baseline parameter for the subsequent determination of activation energies, which can then be used as input parameters for KMC simulations.

2. METHOD

In this study, the MC method with the Metropolis algorithm was employed to analyze the thermodynamic properties of the system, specifically entropy and average energy. The simulation process was carried out using Scilab version 6.1.1. The Lennard-Jones potential, with epsilon (ϵ) and sigma (σ) parameters taken from the literature (Table 1), was used. Only LJ interactions were included; no Coulomb interaction was applied between Li^+ and PF_6^- .

Internal energy (U) can be defined as a state function that can be determined from changes in the entropy and volume of a system. Conjugate variables are pairs of variables associated with changes in internal energy, such as temperature and entropy, as well as pressure and volume. This relationship can be expressed as $dU = T dS - P dV$, where T is temperature, S is entropy, P is pressure, and V is volume. This expression assumes a closed system undergoing a reversible process. In statistical mechanics, a Legendre transformation is applied because it offers advantages in simplifying thermodynamic experiments. By using the variables T and V , experiments can be performed at different temperatures, and the entropy corresponding to those temperatures can be calculated.

Entropy can be regarded as a thermodynamic function that depends on the energy, number of molecules, and volume of a system. Entropy represents a measure of disorder or randomness within the system and can also be calculated using the Boltzmann equation, $S = k \ln \Omega$, where Ω is the number of possible microstates of the system. The distribution of energy quanta in a molecular system provides a means to understand how energy is allocated among the particles in the system. For example, consider a system in which quanta of energy are to be distributed among N particles (atoms or molecules). Each particle may possess a different amount of energy, with several available energy levels ($\epsilon_0, \epsilon_1, \epsilon_2, \dots, \epsilon_M$). The number of ways to achieve a particular distribution can be calculated using a specific formula that accounts for the number of particles occupying each energy level. There are two constraints in this system: (1) The total number of particles occupying the various energy levels must equal the total number of particles N , which can be expressed as $\sum n_j = N$. This means that the total number of particles in the system remains constant. (2) The simulation is performed in the canonical ensemble (N, V, T), where the number of particles N , volume V , and temperature T are kept constant. The system is in thermal contact with a heat bath at temperature T , allowing the total energy $E = \sum n_j \epsilon_j$ to fluctuate. The probability of a microstate is then governed by the Boltzmann distribution. By considering these two constraints, we can determine the distribution of energy quanta in a molecular system and understand how energy is distributed among the particles (Hanson & Green, 2008). This distribution can be described using the Boltzmann distribution, which states that the probability of finding a particle in a particular energy state is proportional to $\exp(-\epsilon_j/k_B T)$.

To maximize Ω , we apply the Stirling approximation and reformulate the problem in terms of maximizing $\ln \Omega$. Stirling's approximation is used to simplify the calculation of multiplicity or entropy for large systems, while the maximum and minimum values are obtained by setting the first derivative equal to zero. Using the Stirling approximation, $\ln \Omega$ can be written as $(\sum n_j) \ln(\sum n_j) - \sum_j n_j \ln n_j$. The problem then becomes maximizing $(\sum n_j) \ln(\sum n_j) - \sum_j n_j \ln n_j$ Subject to the constraints $\sum n_j = N$ and $\sum n_j \varepsilon_j = E$. To solve this constrained optimization problem, we employ the method of Lagrange multipliers, which incorporates the constraints into the function to be maximized through the introduction of Lagrange multipliers (λ). The Lagrange method allows us to maximize a function under specified constraints (Greiner et al., 2012). The Lagrange derivation below is carried out for fixed total energy E (microcanonical); the resulting Boltzmann form is then applied to the canonical ensemble used in the simulation. Using this approach, the expression can be written as follows :

$$\frac{\partial \ln W}{\partial n_j} - \lambda_1 \frac{\partial g_1}{\partial n_j} - \lambda_2 \frac{\partial g_2}{\partial n_j} = 0 \quad (1)$$

After performing the calculations, we can express the equation as:

$$\frac{n_j}{\sum n_j} = \exp(-\lambda_1 - \lambda_2 \varepsilon_j) \quad (2)$$

By applying the constraint $\sum n_j = N$, we can determine the value of λ_1 and express the equation as:

$$\frac{n_j}{\sum n_j} = \frac{\exp(-\lambda_2 \varepsilon_j)}{\sum \exp(-\lambda_2 \varepsilon_j)} \quad (3)$$

Equation (3) represents the Boltzmann distribution, which states that the probability of finding a particle in a given energy state is proportional to $\exp(-\varepsilon_j/k_B T)$ in this equation, λ_2 can be identified as $1/k_B T$, where k_B is the Boltzmann constant, and T is the temperature. Thus, we can understand how the energy distribution in a molecular system can be described using the Boltzmann distribution, allowing us to determine how energy quanta are distributed within the system. If the system has a constant number of molecules, volume, and energy, the distribution of energy quanta can be described using the Boltzmann distribution. A system with a fixed number of molecules, volume, and temperature corresponds to a canonical ensemble. The explicit formulation of the above description is expressed in the following formulation, namely :

$$S = \frac{\bar{E}_p}{T} \quad (4)$$

where $\bar{E}_p$ is the average potential energy. Here $\bar{E}_p$ is the ensemble average of total energy, and in the present Metropolis MC simulation, which samples only configurational degrees of freedom, the directly sampled quantity is the average potential energy $\bar{E}_p$. This expression follows from the high-temperature (classical) limit of the canonical partition function, where entropy scales linearly with the ensemble-averaged energy per degree of freedom (Hanson & Green, 2008).

MC simulations and MD simulations employ different approaches to representing system behavior. MC simulations use statistical methods to generate system configurations that follow the Boltzmann distribution, and the mean potential energy obtained from these configurations is related to the internal energy of the system in a canonical ensemble. In contrast, MD simulations apply Newton's laws to describe the dynamics of the system, allowing the trajectories of particles to be traced from their initial motions and enabling the deterministic calculation of kinetic and potential energy. The distinction between MC and MD lies in their fundamental approaches: MC is stochastic and focuses on sampling system configurations, whereas MD is deterministic and focuses on the time evolution of system dynamics. In MC simulations, the potential energy recorded in the stationary state can be used to compute the thermodynamic properties of the system.

MC simulations can help elucidate the solvation structure of LiPF_6 salt in EC solvent with Vinylene Carbonate additive by sampling molecular configurations according to the canonical (N,V,T) Boltzmann distribution. MC simulations provide insights into the microscopic structure and dynamics

of the system, including solvation phenomena, SEI layer formation, and lithium dendrite growth. Thus, these simulations can help in understanding complex processes at the molecular level and enhance our knowledge of lithium-ion battery systems. However, it should be noted that MC simulations have inherent limitations and rely on certain assumptions, such as the use of accurate potential models and constraints on simulation timescales. Therefore, simulation results must be interpreted with caution and validated against experimental data to ensure their accuracy and reliability.

Table 1 presents a list of several non-bonded force-field parameters used to generate Lennard-Jones interactions. Although the values of ϵ and σ for EC are not explicitly stated as whole-molecule parameters, the ϵ and σ values for the constituent atoms of EC can be found in the table, as is also the case for VC. The parameters for the Li atom are listed separately, while those for the PF_6^- anion, composed of P and F atoms, are also included in the same table.

Table 1. Non-bonded force-field parameters, including epsilon ϵ and sigma σ values for the constituent atoms of EC and VC. The Li atom is listed separately, while PF_6^- consists of P and F atoms.

Atomic pair	Epsilon (ϵ) (kJ/mol)	Sigma (σ) (Å)	Atomic pair	Epsilon (ϵ) (kJ/mol)	Sigma (σ) (Å)
C(sp^3)	0.105	3.75	O	0.170	3.00
C(sp^2)	0.066	3.5	H	0.0030	2.50
O =	0.210	2.96	Li	0.10314	1.4424
F	0.028716	2.9347	P	0.13169	0.18489

However, it should be noted that the overall ϵ and σ values for EC are not explicitly provided in the table. The non-bonded interaction parameters for EC were obtained from the study by Gálvez-Aranda et al. (2017), while the parameters for PF_6^- were taken from the work of Jorn et al. (2013), as presented in Table 1. To calculate the ϵ and σ values for EC, the geometric combining rule for epsilon and the arithmetic combining rule for sigma can be applied (Lahmidi et al., 2025). EC has a molecular structure of $C_3H_4O_3$, consisting of two sp^3 carbon atoms, one sp^2 carbon atom, one carbonyl oxygen, two ether oxygen atoms, and four hydrogen atoms. By using the ϵ and σ values of the constituent atoms of EC, the overall ϵ and σ values for EC can be determined as follows:

$$\epsilon_{EC} = \left(\epsilon(C(sp^3)) \times (\epsilon(C(sp^2)))^2 \times (\epsilon(O=)) \times (\epsilon(O-))^2 \times (\epsilon(H))^4 \right)^{1/10} \quad (5)$$

And sigma (σ) for EC as follows

$$\sigma_{EC} = \frac{(\sigma(C(sp^3)) + 2 \times (\sigma(C(sp^2)))) + (\sigma(O=)) + 2 \times (\sigma(O-)) + 4 \times (\sigma(H))}{10} \quad (6)$$

Thus, the ϵ and σ parameters for the EC molecule are 0.0285 kJ/mol and 2.996 Å, respectively.

The parameters in Table 1 are also used to calculate the epsilon and sigma values for VC (vinylene carbonate), since VC has a molecular structure similar to that of EC. VC has a molecular formula of $C_3H_2O_3$, consisting of three carbon atoms (sp^2 C), two hydrogen atoms, and three oxygen atoms (one carbonyl oxygen and two ether oxygens). Using the parameters provided in the table, the epsilon and sigma values for VC can be calculated in the same manner as previously described.

$$\epsilon_{VC} = \left((\epsilon(C(sp^2)))^2 \times (\epsilon(H))^2 \times (\epsilon(O=))^2 \times (\epsilon(O-)) \right)^{1/7} \quad (7)$$

and the σ for VC is as follows:

$$\sigma_{VC} = \frac{((\sigma(C(sp^2)))) + (\sigma(C(sp^2))) + (\sigma(H)) + (\sigma(H)) + (\sigma(O=)) + (\sigma(O-))}{7} \quad (8)$$

Thus, the ϵ and σ parameters for the VC molecule are 0.0446 kJ/mol and 3.058 Å, respectively.

The ϵ and σ values for the PF_6^- anion were obtained using the geometric combining rule for ϵ and the arithmetic rule for σ , with the epsilon and sigma values for P and F atoms provided in Table 1. The PF_6^- anion has a molecular structure consisting of one phosphorus atom and six fluorine atoms.

$$\varepsilon_{PF_6^-} = \left((\varepsilon(P)) \times (\varepsilon(F))^6 \right)^{1/7} \quad (9)$$

and the σ for PF_6^- is as follows:

$$\sigma_{PF_6^-} = \frac{((\sigma(P)) + 6 \times (\sigma(F)))}{7} \quad (10)$$

The ε value is 0.0357 kJ/mol and the σ value is 2.542 Å for the PF_6^- anion. Thus, by applying the geometric combining rule for epsilon and the arithmetic combining rule for sigma, the atomic and molecular components Li , PF_6^- , EC and VC used for the interaction parameters are presented in Table 2. In the coding process, the researcher used epsilon values in units of *kJ/mol* for atoms and molecules, as shown in Table 3.

Table 2. Cross-species non-bonded LJ parameters (atom–molecule and molecule–molecule pairs) for Li^+ , PF_6^- , EC, and VC.

Atom–molecule pair	Epsilon (kJ/mol)	Sigma (Å)	Molecule–molecule pair	Epsilon (kJ/mol)	Sigma (Å)
$Li - PF_6$	0.2548	1.9887	$PF_6 - EC$	0.1992	2.7530
$Li - EC$	0.3372	2.2067	$PF_6 - VC$	0.2259	2.8335
$Li - VC$	0.3824	2.2872	$EC - VC$	0.2987	3.0515

Table 3. Self and cross-interaction LJ epsilon parameters used in the MC simulation code for Li^+ , PF_6^- , EC, and VC.

Atom–molecule pair	Epsilon (kJ/mol)	Atom–molecule pair	Epsilon (kJ/mol)	Atom–molecule pair	Epsilon (kJ/mol)
$Li - Li$	0.4315	$VC - VC$	0.0810	$Li - VC$	0.3824
$PF_6 - PF_6$	0.1506	$Li - PF_6$	0.2548	$PF_6 - EC$	0.1992
$EC - EC$	0.2636	$Li - EC$	0.3372	$PF_6 - VC$	0.2259
$EC - VC$	0.2987				

The LJ potential with epsilon and sigma parameters taken from previous studies (Jorn et al., 2013) was used to represent interactions between atoms and molecules. The LJ parameters were adopted from previous studies (Jorn et al., 2013; Galvez-Aranda et al., 2017) and were not validated independently in the present study. The simple LJ model neglects polarization, charge transfer, and Coulomb interactions between ions, so the results should be interpreted as a baseline for the employed parameter set and should be tested against experimental or ab initio data in future work. Nevertheless, the simulation has several limitations, including the use of a simple LJ potential and the neglect of polarization effects. Therefore, the results must be interpreted with caution, and further studies are required to improve the reliability of the model (Jorn et al., 2013).

A condition in which a system reaches a stable energy distribution that no longer changes over time is referred to as thermodynamic equilibrium. In MC simulations, thermodynamic equilibrium can be achieved using the Metropolis algorithm, which employs a Markov chain to generate accurate samples that represent the desired probability distribution. A Markov chain is a stochastic process used to model systems that transition randomly from one state to another. In MC simulations, the Markov chain is employed to generate a sequence of states that follows the desired probability distribution. The Metropolis algorithm is an MC method used to generate samples from a specified probability distribution using a Markov chain. This algorithm employs an acceptance criterion to determine whether a proposed atomic displacement is accepted or rejected, based on the transition probability between the old and new states. The acceptance criterion uses the factor $\exp(-\Delta E/kT)$ to determine the probability of accepting the change in atomic position. The Metropolis algorithm enables the generation of accurate samples that represent the desired probability distribution, allowing for precise calculation of the system's properties (Ivan T Dimov, 2008).

The following is a modified flowchart in Figure 1 for the MC simulation code involving four species: Li^+ , PF_6^- , EC, and VC. (A) Initialization: (A1) Determine the number of atoms for each type (Li^+ , PF_6^- , EC, and VC). (A2) Set the box size (L). (A3) Specify the temperature (T) and the

universal gas constant (R). (A4) Define the L J parameters for each atom–molecule and molecule–molecule pair ($\text{Li}^+ - \text{Li}^+$, $\text{Li}^+ - \text{PF}_6^-$, $\text{Li}^+ - \text{EC}$, $\text{Li}^+ - \text{VC}$, $\text{PF}_6^- - \text{PF}_6^-$, $\text{PF}_6^- - \text{EC}$, $\text{PF}_6^- - \text{VC}$, $\text{EC} - \text{EC}$, $\text{EC} - \text{VC}$, and $\text{VC} - \text{VC}$). (A5) Randomly initialize the positions of atoms and molecules for each type. (B) MC Simulation: Perform the iterations for the specified number of steps. (B1) Randomly select an atom or molecule from any type. (B2) Randomly update the position of the selected atom or molecule. (B3) Calculate the new potential energy by considering the interactions between the selected particle and all other atoms and molecules. (B4) Compute the change in energy. (B5) Accept or reject the new position based on the Boltzmann probability. (B6) Update the average potential energy. (B7) Store the average potential energy value. (B8) Check if the maximum number of MC steps has been reached. If not (No), return to B1 to select a new atom or molecule at random for the next trial move. If yes (Yes), terminate the simulation. (C) Visualization: (C1) Visualize the initial and final positions of the atoms for each type. (C2) Visualize the average potential energy versus the number of steps. MC simulations were performed using the default random number generator in Scilab without an explicitly set random seed value, i.e., `rand()` was used for particle displacement and acceptance.

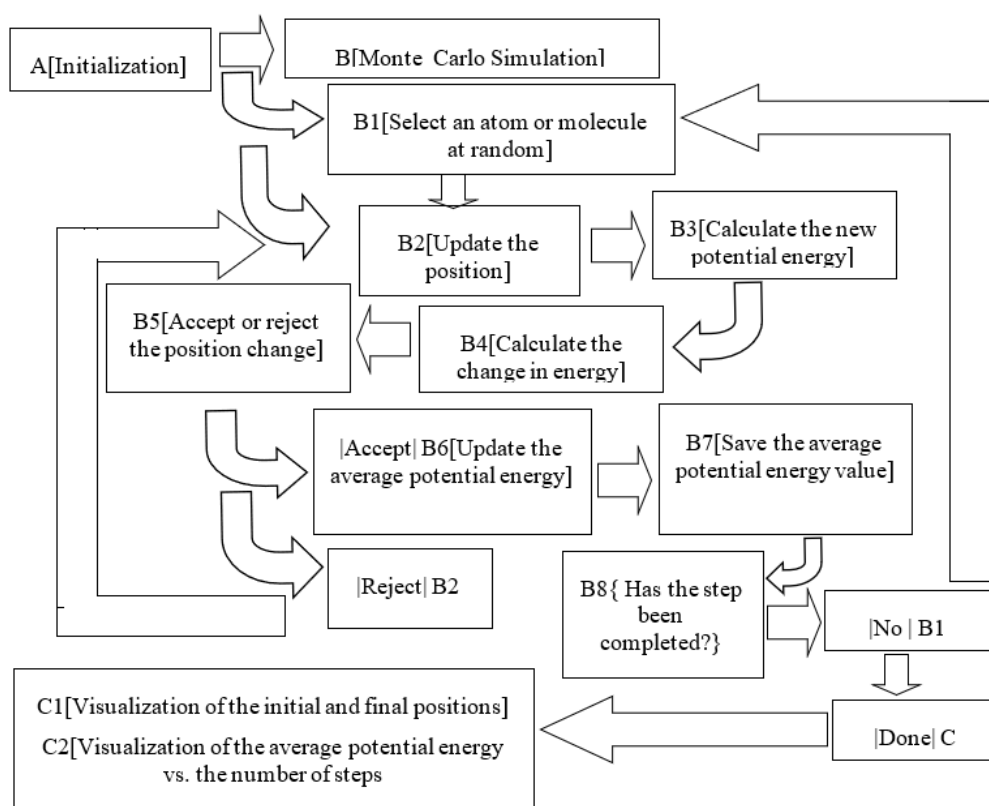


Figure 1. Flowchart for the MC simulation code for four species: (A) Initialization. (B) MC simulation, performed for the specified number of iterations. (C) Visualization.

The method used in this study to test convergence, as shown in Figure 6, is the cumulative average method. This method evaluates convergence by plotting the cumulative average energy as a function of time (simulation steps). If the simulation has converged, the cumulative average energy becomes stable and does not change significantly as the number of steps increases. The cumulative average energy is calculated by summing all energy values at each simulation step and dividing by the total number of steps. The resulting plot of cumulative average energy versus time can be used to assess convergence, and as observed, for the green curve, the simulation has converged, and the average energy value is valid. Uncertainty was estimated as the standard error of the cumulative average, and the standard deviation was calculated from the spread of instantaneous energy values around the cumulative mean. In this study, a simulation was operationally defined as having reached thermodynamic equilibrium when the ratio of this uncertainty estimate to the standard deviation fell below 10%. This

criterion was satisfied only for the 400-particle, $L = 200 \text{ \AA}$, 100,000-step condition (Figure 5). Reaching this criterion indicates equilibration of the sampled ensemble but does not, by itself, demonstrate that the corresponding configuration is a global energy minimum, since standard Metropolis Monte Carlo samples the canonical ensemble without performing global optimization (e.g., simulated annealing or basin-hopping).

3. RESULTS AND DISCUSSION

The results of the MC simulations are presented in Figures 2 and 3. The ε and σ data were taken from Table 3. Figure 2 shows the simulation of the solvation events involving the LiPF_6 salt, the solvent ethylene carbonate $(\text{CH}_2\text{O})_2\text{CO}$, and the additive Vinylene Carbonate $(\text{C}_3\text{H}_2\text{O}_3)$. The total number of particles used in the simulation was 200, consisting of 50 each of Li^+ ions, PF_6^- ions, EC molecules, and VC molecules. The initialization of atomic positions was performed using a specific script, in which the most important part is the box size defined in the simulation, as shown in Figure 2. In this study, the researcher selected a box length of $L = 60 \text{ \AA}$. This means that the program randomly distributed the initial positions of the Li^+ , PF_6^- , $(\text{CH}_2\text{O})_2\text{CO}$, and $\text{C}_3\text{H}_2\text{O}_3$ within a $60 \text{ \AA}$ range. A larger value of L results in a larger interatomic distance r within the Lennard-Jones potential, which in turn decreases the average potential energy. The temperature used in the simulation was 300 K. The simulation conditions in Figure 3 were identical to those in Figure 2, except that the number of simulation steps was increased to 100000 to improve system convergence and stability.

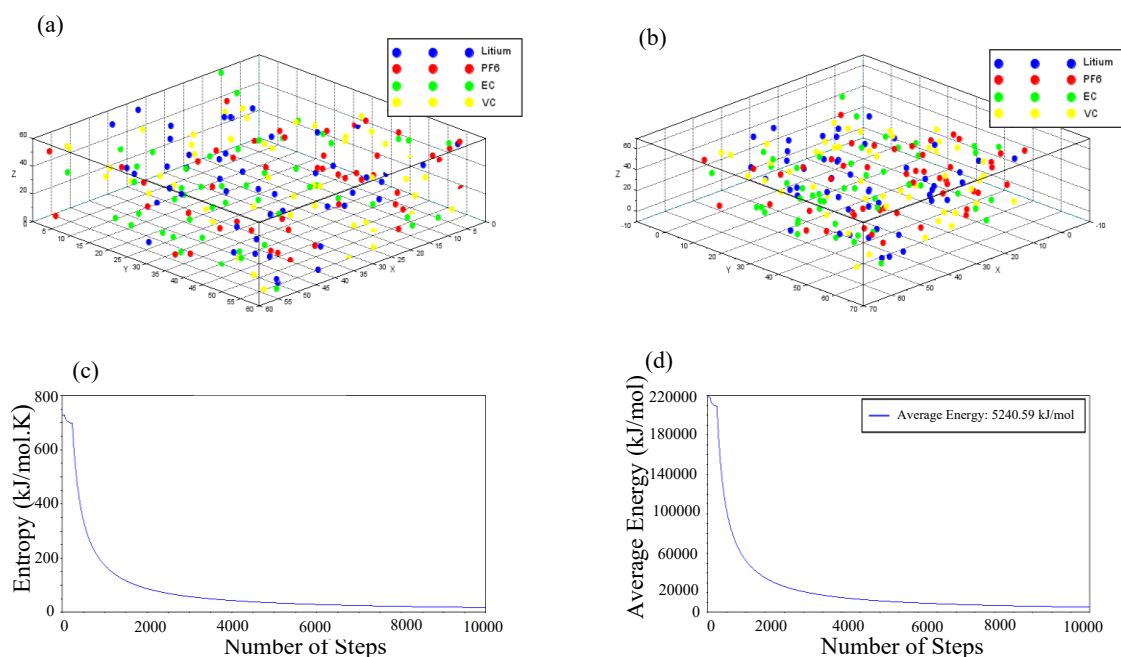


Figure 2. MC evolution for 200 particles (50 each of Li^+ ions, PF_6^- ions, EC molecules, and VC molecules) in a cubic box of length L : (a) initial configuration, (b) configuration after 10000 steps, (c) entropy vs. MC steps, and (d) running average LJ potential energy vs. MC steps. The energy trace indicates the system has not yet reached equilibrium.

A negative average energy indicates that the Lennard–Jones (LJ) potential between the atoms or molecules in the system is attractive, which is a typical characteristic of the LJ potential, a mathematical model used to describe interactions between atoms or molecules. This potential consists of two components: an attractive component (London dispersion forces) and a repulsive component (Pauli repulsion). The LJ potential can be expressed as:

$$V(r) = 4\varepsilon \left(\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right) \quad (11)$$

where ϵ is the potential-well depth, σ is the characteristic distance at which the potential is zero, and r is the interatomic or intermolecular distance. If the average energy is negative, it indicates that the LJ potential between the atoms or molecules is attractive and sufficiently strong for them to remain together and form a stable structure. A negative value of the average LJ potential indicates that attractive contributions dominate over repulsive contributions relative to the zero of the potential. The attainment of thermodynamic equilibrium was assessed separately from the energy sign, based on the convergence of the average potential energy with respect to MC steps. Conversely, a positive average energy corresponds to a repulsive LJ potential, causing the atoms or molecules to move apart.

Figure 2 shows that after 10000 MC steps (~ 1 h), the running average energy was 5240.59 kJ/mol. Extending the simulation to 100000 steps (~ 6 h, Figure 3) lowers the running average to 522.77 kJ/mol and shows a flatter energy trace. This indicates that 10000 steps were insufficient for equilibration. Equilibrium was assessed from the convergence of the running average potential energy [Figure 3]. We do not claim that the configuration corresponds to the global minimum, as standard Metropolis MC samples the canonical ensemble and does not guarantee global optimization.

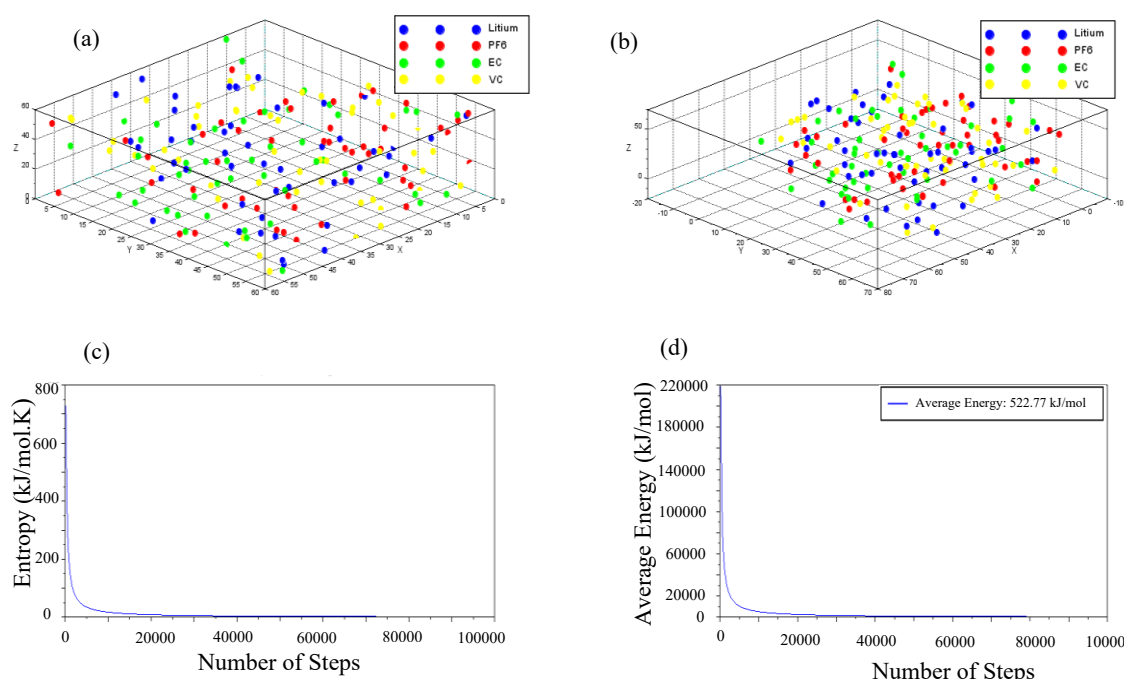


Figure 3. Solvation of LiPF_6 salt, $(\text{CH}_2\text{O})_2\text{CO}$, and the additive $\text{C}_3\text{H}_2\text{O}_3$ interacting. The total number of particles is 200, with 50 each of Li^+ , PF_6^- , $(\text{CH}_2\text{O})_2\text{CO}$, and $\text{C}_3\text{H}_2\text{O}_3$. The box size, L , is an important parameter. (a) Initial positions of atoms and molecules, (b) final positions of atoms and molecules, (c) entropy versus step number (100000), and (d) average energy versus number of steps. The running average had not yet converged, indicating the system had not yet reached thermodynamic equilibrium.

Figure 4 shows that when the simulation was run for 10000 steps with an execution time of approximately three hours, the resulting average energy was 0.25 kJ/mol. The difference compared to Figure 2 lies in the number of particles: the total number of particles is 400, with 100 each of Li^+ , PF_6^- , $(\text{CH}_2\text{O})_2\text{CO}$, and $\text{C}_3\text{H}_2\text{O}_3$. Another difference from Figure 2 is the box size, where the researcher chose $L = 200$ Å. The initial positions of the Li^+ , PF_6^- , $(\text{CH}_2\text{O})_2\text{CO}$, and $\text{C}_3\text{H}_2\text{O}_3$, 100 particles each were randomly distributed within the 200 Å range. A larger value of L results in a greater interatomic distance r in the Lennard-Jones potential, which affects the average energy value. The running average energy had not yet converged after only 10000 steps, indicating that thermodynamic equilibrium had not yet been reached. A longer simulation was expected to allow the system to approach a more stable, lower-energy configuration. Nevertheless, the average energy is already significantly lower than in the previous simulation. In the previous simulation shown in Figure 2, the average energy was 5240.59 kJ/mol, whereas in this simulation it is only 0.25 kJ/mol.

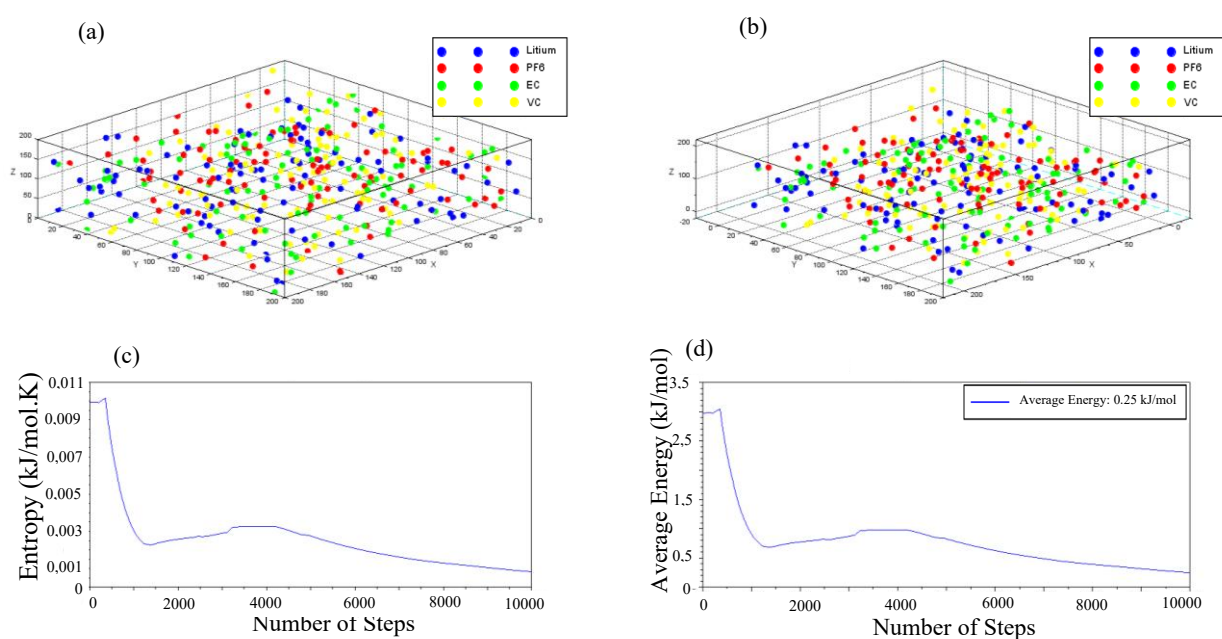


Figure 4. Solvation of LiPF₆ salt, (CH₂O)₂CO, and the additive C₃H₂O₃ interacting. The total number of particles is 400, with 100 each of Li⁺, PF₆⁻, (CH₂O)₂CO, and C₃H₂O₃. The box size, L, is larger than in the previous figure, at 200 Å. (a) Initial positions of atoms and molecules, (b) final positions of atoms and molecules, (c) entropy versus number of steps (10000), and (d) average energy versus number of steps. The running average had not yet converged, indicating the system had not yet reached thermodynamic equilibrium; however, the average energy is significantly lower than in the previous simulation, at 0.25 kJ/mol.

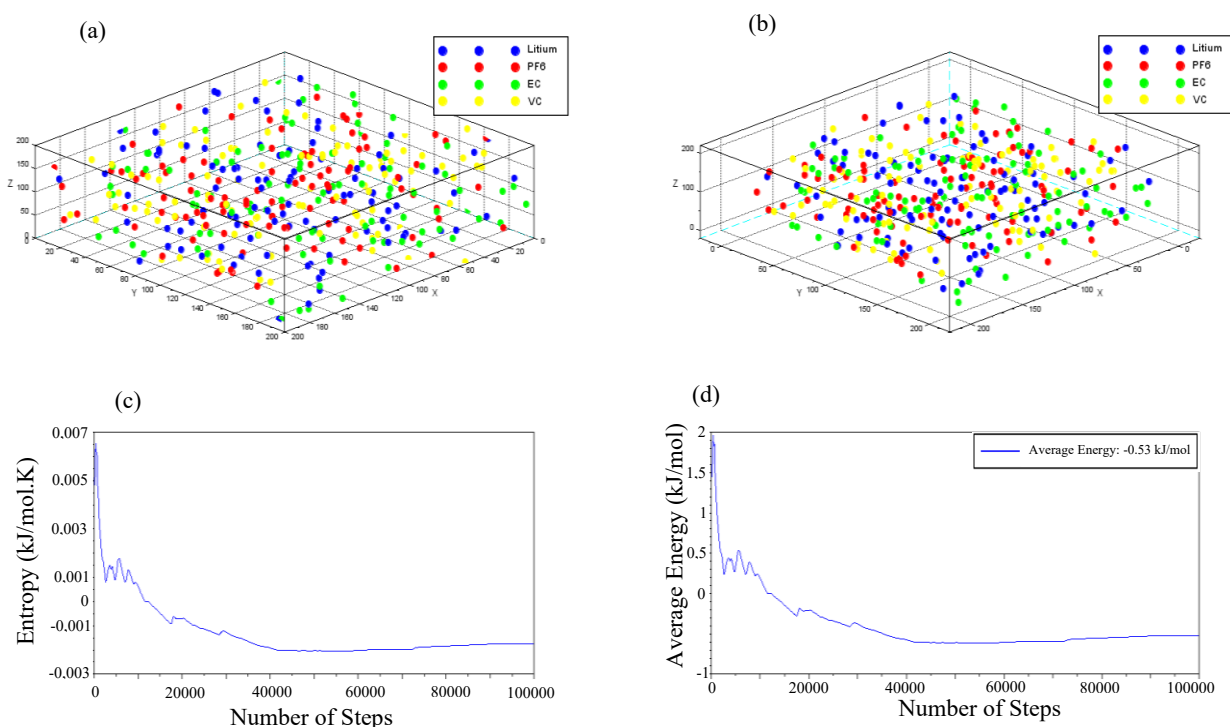


Figure 5. Solvation of LiPF₆ salt, EC, and VC additive (400 particles total, 100 each of Li⁺, PF₆⁻, EC, and VC; L = 200 Å): (a) initial configuration, (b) final configuration after 100000 MC steps, (c) entropy vs. number of MC steps, and (d) running average LJ potential energy vs. number of MC steps. The system approaches equilibrium with a running average of -0.53 kJ/mol.

Figure 5 shows that when the simulation is run for 100000 steps with an execution time of over 12 hours, the resulting average energy is -0.53 kJ/mol. The difference compared to Figures 2 and 4 lies in the number of steps, which is 100000 in this simulation. The number of particles for each type Li , PF_6 , $(CH_2O)_2CO$, and $C_3H_2O_3$ is 100. The box size is $L = 200$ Å. The initial positions of the atoms Li , PF_6 , $(CH_2O)_2CO$, and $C_3H_2O_3$ were randomly distributed within the 200 Å range. A larger value of L results in a greater interatomic distance r in the Lennard-Jones potential, which affects the average energy value. The convergence criterion defined in the Method section (uncertainty-to-standard-deviation ratio below 10%) was satisfied for this simulation, indicating that thermodynamic equilibrium had been reached. This does not imply that the configuration corresponds to a global energy minimum, since the Metropolis MC method used here does not perform a global search; however, the average energy is significantly lower than in the previous simulations, where the average energies were 5240.59 kJ/mol and 0.25 kJ/mol, whereas in this simulation, it is -0.53 kJ/mol. The running average LJ potential energy reflects cohesive interactions in the simulated mixture; a more negative value indicates stronger net attraction under the employed LJ parameters. No activation barriers were calculated in this MC study, so no inference about reactivity is made. Determination of activation energies would require explicit transition-state calculations.

Four MC simulations were performed for the $LiPF_6$ electrolyte system in a mixed solvent of EC and VC with variations in the number of particles (200 and 400), box size ($L = 100$ Å and 200 Å), and number of MC steps (10000 and 100000), as shown in Figures 2–5. In the first simulation, consisting of 200 particles in a 60 Å box with 10000 steps, the system contained 50 Li^+ ions, 50 PF_6^- ions, 50 $(CH_2O)_2CO$ molecules, and 50 $C_3H_2O_3$ molecules randomly distributed within the simulation box. The obtained average energy was relatively high, at 5240.59 kJ/mol, because the short interparticle distances caused the repulsive component of the Lennard–Jones potential to become dominant. In the second simulation, the number of each species was increased to 100, resulting in a total of 400 particles, and the box size was enlarged to 200 Å while maintaining the same 10000 simulation steps. The average energy decreased drastically to 0.25 kJ/mol because the larger box increased the interparticle distance r , thereby reducing the Lennard–Jones potential $V(r)$. However, under these conditions, the system had not yet reached thermal equilibrium. The third simulation used the same parameters as the second simulation, but the number of steps was extended to 100000. The average energy became -0.53 kJ/mol. This negative value indicates that the attractive Lennard–Jones interactions became dominant, and the convergence of the cumulative average (Table 4) indicates that the system had reached thermodynamic equilibrium under the simulated conditions. From these four simulations (Figures 2–5), it can be concluded that the average LJ potential energy is influenced by system density through the interparticle distance r in the Lennard–Jones potential. Increasing the box size L at fixed particle number lowers the particle density and reduces repulsive contributions, whereas extending the number of MC steps allows the running average to converge toward equilibrium, as seen by the more negative value in Figure 5.

The quantity calculated in this work is the running average Lennard–Jones potential energy of the electrolyte mixture. No chemical reaction or transition state was simulated, and no activation barriers were determined. Assessment of reactivity would require separate transition-state search or free-energy barrier methods, which are beyond the scope of the present MC study. Although the average potential energy is expected to relate to reactivity and SEI formation in future KMC modeling, establishing that relationship quantitatively is left for future work using the transition-state methods noted above. In the context of lithium battery performance, a low average energy promotes the formation of the SEI layer and the growth of lithium dendrites as reaction products, which in turn accelerates battery aging and reduces cycle life.

Figure 6 shows simulations of the solvation process of the $LiPF_6$ salt and the ethylene carbonate $((CH_2O)_2CO)$ solvent, along with the Vinylene Carbonate $(C_3H_2O_3)$ additive. The total number of particles is 200, where each species— Li^+ , PF_6^- , $(CH_2O)_2CO$, and $C_3H_2O_3$ consists of 50 particles. Figure 6 is included as a negative control to illustrate the importance of choosing a proper box size. At $L = 10$ Å the system is highly overlapped, leading to divergence of LJ energy to $\sim 10^6$ kJ/mol. This case is not used for production analysis; all production runs use $L = 60$ Å (1.53 M), as in Figures 2–3.

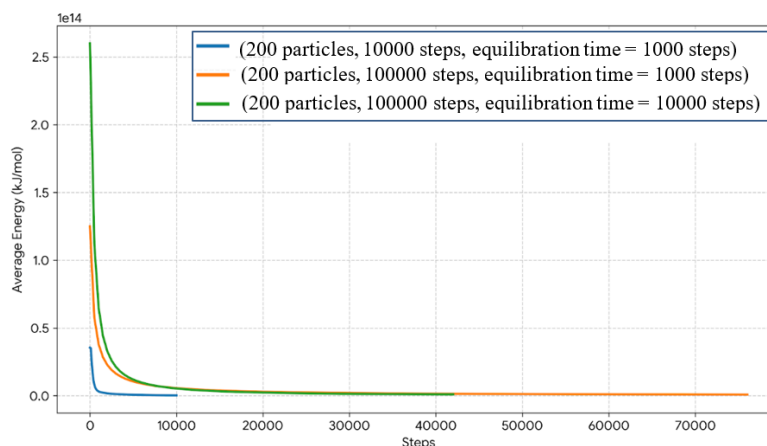


Figure 6. Effect of box size on energy convergence. Demonstration of the unphysical overlap regime at $L = 10$ Å (332 M) vs. the normal regime at $L = 60$ Å.

Table 4 shows that the estimated error for the blue curve, the standard deviation, is still too large; therefore, the researcher cannot confirm whether the simulation has converged. The standard deviation is typically larger than the uncertainty estimate because the standard deviation measures how much the data fluctuate around the mean, whereas the uncertainty estimate measures the possible error in the estimated mean.

Table 4. Cumulative average energy statistics for the three convergence-test conditions shown in Figure 6.

Colour	Steps	Equilibration time (steps)	Average energy (kJ/mol)	Minimum energy (kJ/mol)	Maximum energy (kJ/mol)	Uncertainty estimation	Standard deviation
Blue	10000	1000	936965	2148	35971520	104079	3155389
Orange	100000	1000	38177	-59	4122487	2610	259993
Green	100000	10000	30.20	-75	2003.50	7.30	219

Table 5. Convergence assessment summary for the three box-size conditions in Figure 6.

Colour	Data description (Uncertainty)	Error estimation	Data description (error estimation)
Blue ($L=10\text{Å}$)	The estimated uncertainty value is smaller than the standard deviation, the simulation has not converged.	1127373	The error estimate is smaller than the standard deviation; the calculation results are quite accurate.
Orange ($L=60\text{Å}$)	The estimated uncertainty value is smaller than the standard deviation, the simulation has not converged.	72340	The error estimate is smaller than the standard deviation; the calculation results are quite accurate.
Green ($L=60\text{Å}$)	The estimated uncertainty value is smaller than the standard deviation, the simulation has converged.	98	The error estimate is smaller than the standard deviation; the calculation results are quite accurate.

The orange and green curves show simulations performed with 100000 steps, presenting a plot of the cumulative average energy as a function of the simulation step, which illustrates how the average energy changes as the number of simulation steps increases. For the orange curve, the standard deviation decreases compared to the previous case; however, the researcher still cannot confirm whether the simulation has converged. For the green curve, the standard deviation, uncertainty estimate, and error estimate are smaller than in the two previous simulations; therefore, the researcher assumes that the simulation has converged. Convergence was assessed from the cumulative average plot (Figure 6, see Methods for definition). The convergence ratio for the green curve is calculated from an uncertainty estimate of 7.30 kJ/mol divided by a standard deviation of 219 kJ/mol, yielding a value of 0.033 or

3.3%. This value satisfies the explicit convergence criterion, i.e., the standard error is less than 10% of the standard deviation, so the green simulation is declared to have converged. The green curve in Table 5 is stated as converged with $SE = 7.30 \text{ kJ/mol}$, which is equivalent to 3.3% of the standard deviation of 219 kJ/mol .

For comparison, the present average-energy values were compared with those obtained by other researchers who used Molecular Dynamics to observe the behavior of Na^+ ions in $\text{NaPF}_6/\text{DMSO}$ electrolytes at various temperatures. The results showed that the average energy at 298.15 K was $2.53 \times 10^4 \text{ kJ/mol}$, at 313.5 K was $2.66 \times 10^4 \text{ kJ/mol}$, at 353.15 K was $3 \times 10^4 \text{ kJ/mol}$, and at 373.15 K was $3.17 \times 10^4 \text{ kJ/mol}$ (Chliyah et al., 2026). The results reported by other researchers indicate that the average energy of the KPF_6/DMSO system over the temperature range of $300\text{--}400 \text{ K}$ increased from 3.0×10^4 to $3.3 \times 10^4 \text{ kJ/mol}$ (Callegari et al., 2025). Increasing temperature weakens the ion solvent interactions and strengthens the ion–ion interactions, leading to the formation of contact ion pairs, which increases the mobility of Na^+ ions because the ions can more easily escape from the solvation shell. These results help determine the operating temperature and solvent selection in order to maintain high conductivity without excessively increasing viscosity. On the other hand, the researchers used the MC method to evaluate the stability of the LiPF_6 system in a mixed EC and VC solvent, which are additives commonly used in commercial lithium-ion batteries. The simulation results showed that when the box size was enlarged and the number of simulation steps was increased, the system reached a stable negative potential energy. This negative energy indicates the presence of dominant attractive interactions among the components, causing the electrolyte structure to tend toward a thermodynamically stable state. This finding explains at the molecular level why VC is effective in forming a compact SEI layer and protecting the anode from further degradation. This study also provides important insights into the simulation methodology itself. When the simulation box is too small, or the number of steps is insufficient, the system can easily become trapped in a local energy minimum, causing the results to fail to represent the actual conditions. Therefore, these findings serve as a guideline for other researchers to ensure that *Li-ion* electrolyte simulation settings produce valid data. With this stability information, new electrolyte formulations can be screened more rapidly without requiring extensive laboratory experiments.

The differences in the average energy values among Figures 2, 3, 4, and 5 are closely related to the simulation box size and simulation time employed. When the box size was increased from $60 \text{ \AA}$ (Figures 2 and 3) to $200 \text{ \AA}$ (Figures 4 and 5), the system volume increased substantially, resulting in a significant decrease in particle density. In the LJ potential, the interaction energy strongly depends on the distance between particles. As the average interparticle distance increases, both the short-range repulsive interactions and the long-range van der Waals attractive interactions become very weak, causing the total potential energy of the system to approach zero. This is evident from the decrease in the average energy from 5240.59 kJ/mol (Figure 2) to 0.25 kJ/mol (Figure 4). The negative energy value of -0.53 kJ/mol in Figure 5 indicates that, with a longer simulation time of 100000 steps, the system had sufficient time to approach equilibrium, allowing attractive intermolecular interactions to be more effectively established. Therefore, the decrease in average energy can be attributed to the weakening of interparticle interactions as the average distance between particles increases, together with the achievement of a more equilibrated state during the longer simulation.

4. CONCLUSION

This study simulated the $\text{LiPF}_6/\text{EC}/\text{VC}$ electrolyte system using four MC simulations with different numbers of particles, simulation box sizes, and MC steps. The average energy decreased from 5240.59 kJ/mol to 0.25 kJ/mol as the simulation box size increased, owing to the greater intermolecular distances, which reduced the Lennard-Jones repulsive interactions. By increasing the number of MC steps, the average energy further decreased to -0.53 kJ/mol , indicating that the system had approached convergence, as evidenced by the stabilization of energy fluctuations, where attractive interactions became dominant. The reductions in the standard deviation, uncertainty, and estimation

error, together with the stability of the cumulative average, demonstrate that the simulation had converged, confirming the validity of the calculated average energy.

The previous study and the present study complement each other in the development of battery electrolytes. The previous study employed MD simulations to investigate the dynamics of Na^+ ions in a $NaPF_6/DMSO$ electrolyte and found that increasing temperature weakened the $Na^+ - DMSO$ interactions while strengthening the $Na^+ - PF_6^-$ interactions, leading to the formation of contact ion pairs that enhanced ion mobility. These findings are relevant for determining the optimal operating temperature and selecting suitable solvents to achieve high ionic conductivity without excessive viscosity. In contrast, the present study employed MC simulations to evaluate the stability of the $LiPF_6$ electrolyte in an EC/VC solvent system. By increasing the simulation box size and the number of MC steps, the system reached a stable negative potential energy, indicating that attractive intermolecular interactions became dominant and that the electrolyte structure was thermodynamically stable. These results provide a molecular-level explanation of the role of VC in promoting the formation of a dense and stable solid electrolyte interphase (SEI). Overall, the previous study focused on ion dynamics and transport, which influence power density and charging rate, whereas the present study emphasizes structural stability and thermodynamic behavior, which are closely related to battery safety and cycle life. Together, these two computational approaches reduce the need for extensive experimental trial-and-error and accelerate the optimization of electrolyte formulations by providing a clearer molecular-level understanding.

Each condition was simulated only once without setting an explicit random seed and without replication using different random seeds. Consequently, statistical uncertainty could not be assessed, and reproducibility is limited. Future work should set and report explicit random seeds and perform multiple independent replicates.

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AUTHOR CONTRIBUTIONS

Conceptualization, E.S. and H.N.; methodology, E.S. and H.N.; investigation, E.S.; formal analysis, E.S. and H.N.; data curation, E.S.; writing-original draft preparation, E.S.; writing-review and editing, E.S. and H.N.; visualization, E.S.; supervision, H.N. All authors have read and agreed to the published version of the manuscript.

CONFLICTS OF INTEREST

The authors declare no conflict of interest.

ARTIFICIAL INTELLIGENCE (AI) USAGE DECLARATION

During the preparation of this work, the authors used ChatGPT (OpenAI) for language improvement, translation, and assistance in organizing the manuscript. After using this tool, the authors reviewed and edited the output as needed and took full responsibility for the content of the publication. Translate.

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