Joint Institute for Nuclear Research

Laboratory of Nuclear Problem

Final Report on the INTEREST Program

Introductory Course: MD-Simulation Research (From Atomic Fragments to Molecular Compound)

Supervisor: Prof Kholmirzo Kholmurodov

(Frank Laboratory of Neutron Physics)

Student: Aadhyatri Pathak

(Institute of Chemical Technology, Mumbai)

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Abstract

This report provides a brief and systematic study on the use of Molecular Dynamics (MD) simulations to understand atomic-scale behavior in solid-state electrolyte materials. The work builds on the theoretical principles and modeling strategies presented in the lectures and in the literature edited by Dr. Kholmirzo Kholmurodov. These sources emphasize how nanoscale processes influence the structural, transport, and functional properties of both biological and inorganic systems.

For this project, an atomistic model of a lithium-based solid electrolyte was created and examined. The goal was to observe lithium-ion movement within the crystal lattice and to assess how the local coordination environment, lattice vibrations, and structural differences affect ionic mobility. Using classical MD techniques, key transport metrics such as ion paths, radial distributions, mean square displacement (MSD), and basic diffusion characteristics were evaluated during the simulation.

Although the study is introductory, it offer valuable insight into the link between microscopic ionic motion and macroscopic material performance, especially in terms of conductivity, stability, and ion-transport directionality in solid electrolytes. The project also provided hands-on experience with selecting force fields, setting simulation parameters, conducting system relaxation, and interpreting data. This reinforced the basic concepts discussed in Dr. Kholmurodov's work on nanoscale modeling. Overall, the study shows how MD simulations serve as an effective tool for analyzing and predicting the behavior of advanced materials. It also highlights their importance in designing and optimizing next-generation solid-state battery components.

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1. Introduction

Molecular Dynamics (MD) is a computational method for studying atomic and molecular motion by numerically integrating Newton's equations of motion. By assigning positions, velocities, and interaction potentials to atoms, MD produces detailed trajectories that show how a molecular system changes over time. This method gives insights into structural, thermodynamic, and dynamic behavior, complementing experimental techniques like X-ray crystallography, neutron scattering, and NMR spectroscopy. MD connects microscopic interactions to macroscopic observations, allowing the extraction of properties such as energy, pressure, diffusion coefficients, and relaxation behavior through time-averaged measurements.

The foundations of MD were established in the 1950s by Alder and Wainwright through hard-sphere simulations, showing how computational methods could imitate atomic interactions. A significant breakthrough happened in 1964 when Rahman conducted the first realistic MD simulation of liquid argon using continuous interatomic potentials. Verlet later introduced an efficient integration algorithm, which improved numerical stability and reduced computational costs. These advances changed MD from a conceptual method into a widely used tool in materials science, chemistry, and biological research.

MD is closely linked to statistical mechanics, which provides the theoretical framework to connect microscopic atomic motion with macroscopic thermodynamic properties. Using the Boltzmann distribution and ensemble theory, MD simulations can calculate temperature, pressure, heat capacities, and structural correlations like radial distribution functions. Equilibrium simulations require sufficiently long trajectory sampling, while non-equilibrium MD allows for the modeling of thermal conductivity, viscosity, and external disturbances.

Modeling the motion of a complex molecule by explicitly solving the wave functions of all subatomic particles would give the most accurate description of molecular behavior. This is achieved through the time-independent Schrödinger equation:

$$\frac{h^2}{2m}\nabla 2\psi + U(x,y,z)\Psi(x,y,z) = E\Psi(x,y,z)$$

However, solving this equation for systems containing hundreds or thousands of atoms is extremely difficult to program and far beyond feasible computational limits. For this reason, full quantum-mechanical treatments are restricted to small molecules or short-timescale processes.

To study larger systems, classical Newtonian mechanics is employed in Molecular Dynamics (MD) as a simplified but computationally efficient alternative. Although classical MD does not explicitly account for electronic transitions, bond breaking, or charge redistribution, it uses force fields, empirical or semi-empirical functions derived partly from quantum mechanical calculations to approximate interatomic forces. This allows the simulation of systems containing tens of thousands of atoms over nanosecond to microsecond timescales. Thus, MD represents a practical compromise between physical accuracy and computational tractability, retaining essential quantum-derived information while enabling large-scale simulations that are otherwise impossible.

Numerical values obtained from quantum chemistry calculations are incorporated into classical potential energy functions, helping bridge the gap between quantum accuracy and classical efficiency.

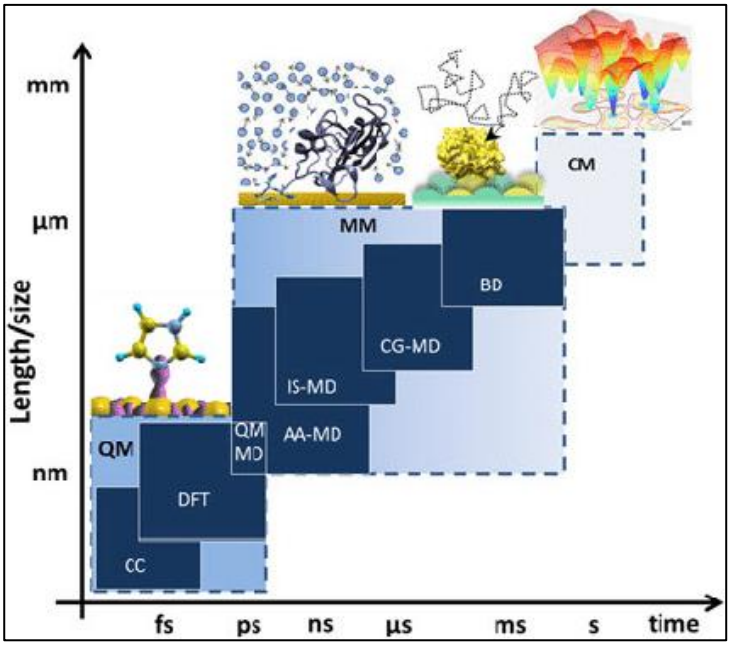

Figure 1 Typical time and length scales of different simulation techniques

The figure shows the typical time and length scales related to different computational simulation techniques. It demonstrates that quantum mechanical methods work on the smallest scales, while atomistic molecular dynamics (MD) operates at intermediate scales. Coarse-grained or continuum models cover larger spatial and temporal areas. In atomistic simulations, the main goal is to accurately capture how individual atoms move and interact within a material. By understanding how these atoms behave collectively, we can gain insight into larger phenomena like deformation, phase changes, and structural transformations. However, extracting trustworthy information from atomic trajectories can be difficult due to issues with vibrations,

spatial rearrangements, connecting changes, and dynamic fluctuations. One strong point of MD simulations is their capability to reveal dynamic properties. These include transport coefficients, time-dependent responses, flow behavior, and vibrational patterns. MD connects microscopic motion to observable macroscopic effects, serving as a link between atomic-scale processes and laboratory experiments. For instance, we can get diffusion coefficients from velocity autocorrelation functions, while structural order can be derived from radial distribution functions. MD also offers a useful platform for testing theoretical models by allowing direct comparison between simulation results and experimental data. Additionally, it lets researchers explore extreme conditions, such as high temperatures, high pressures, or nonequilibrium states, which may be hard or impossible to replicate in experiments. While MD lowers empirical assumptions by using quantum-derived forces, it is still limited to relatively small systems because of its high computational cost. In many situations, simpler classical models that capture just the essential physics are enough to differentiate between competing theories and study large-scale phenomena. Overall, molecular dynamics provides a strong and clear framework for examining the behavior of biomolecules, materials, and complex chemical systems. It offers insights that are crucial for understanding their structure, function, and interactions.

2. Fundamental Equations and Interaction Potentials

Molecular Dynamics (MD) relies on the mathematical framework of classical mechanics and the accurate representation of interatomic potentials to describe how atoms behave over time. These two components' equations of motion and interaction potentials form the core of every MD simulation.

2.1 Newton's Equations of Motion

At the foundation of MD lies Newton's Second Law, which relates the force acting on a particle to its mass and acceleration.

For each atom *i* in a system of *N* atoms:

$$F_i = mi \left(\frac{d^2 r_i}{dt^2}\right)$$

The force on each atom is obtained from the negative gradient of the potential energy surface:

$$F_i = -\nabla i \, U(r)$$

Molecular dynamics simulations advance the positions and velocities of atoms by numerically integrating these equations of motion using extremely small-time steps, typically on the order of 1-2 femtoseconds. This fine temporal resolution generates detailed trajectories that capture

the evolving positions, velocities, and accelerations of all particles, enabling the evaluation of thermodynamic and dynamic properties. To achieve this, several integration schemes are commonly employed: the Verlet algorithm, known for its simplicity and robustness; the Velocity Verlet method, which updates positions and velocities simultaneously for improved accuracy; and the Leapfrog method, valued for its excellent long-term energy conservation. The selection of an appropriate integrator plays a crucial role in determining the overall stability, precision, and computational efficiency of the simulation.

2.2 Potential Energy Components

The potential energy function, commonly known as the force field, dictates how atoms interact. It is composed of bonded and non-bonded interactions:

$$\boldsymbol{U_{total} = U_{bonded} + U_{nonbonded}}$$

Each term governs a different aspect of molecular behaviour, from internal structural constraints to long-range forces.

- **Non-Bonded Interactions:** Non-bonded forces arise between atoms that are not directly linked by covalent bonds and play a critical role in shaping macroscopic behaviour such as protein folding, molecular self-assembly, surface interactions, and solvation phenomena. The primary contributors to these interactions are van der Waals forces and electrostatic (Coulombic) interactions, both of which operate across numerous atom pairs and therefore impose significant computational demands in molecular dynamics simulations.

$$U_{nonbonded} = U_{LJ} + U_{elec}$$

To manage this complexity, efficient neighbour-list constructions and cutoff schemes are implemented to limit calculations to only the most relevant interacting pairs, thereby improving performance without compromising accuracy.

- **Van der Waals Forces:** Van der Waals interactions originate from temporary dipoles and small charge fluctuations that occur as electrons move within and between atoms. Although individually weak, these forces collectively influence the structure, stability, and behaviour of molecular systems

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

In MD simulations, they are commonly represented using the Lennard-Jones (LJ) potential, which accounts for strong repulsion at very short distances and gentle attraction at moderate

ranges. This balance allows the LJ model to realistically describe molecular packing, steric effects, and the overall cohesion observed in liquids, soft materials, and condensed phases.

- **Electrostatic Interactions** Electrostatic interactions between charged or partially charged atoms are long-ranged and decay slowly with distance, as described by Coulomb's Law.

$$U_{elec}(r) = \frac{q_i q_j}{4\pi\varepsilon_0 r}$$

These forces strongly influence hydrogen bonding, ionic stability, and solvation behavior. Because simple cutoffs cause large errors, modern MD simulations use techniques such as Ewald Summation and Particle Mesh Ewald (PME), which accurately and efficiently handle long-range electrostatic interactions by splitting the calculation into real-space and reciprocal-space components.

- **Combined Non-Bonded Potential:** Most force fields represent non-bonded interactions using a combination of Lennard-Jones and Coulombic terms, offering a balanced and comprehensive description of how atoms influence one another at short and long ranges. This combined approach effectively captures van der Waals forces, steric repulsion, and electrostatic attractions, making it essential for accurately modelling the behaviour of liquids, biomolecules, polymers, and nanomaterials.

- **Bonded Interactions:** Bonded interactions play a crucial role in preserving the internal geometry of molecules by constraining how atoms move relative to one another. They encompass bond stretching, which describes the vibrational motion between two covalently connected atoms; angle bending, which governs changes in the bond angle formed by three atoms and dihedral or torsional motion, which involves rotation around covalent bonds and determines the relative orientation of connected atomic groups. Together, these bonded interactions ensure that molecular conformations remain physically realistic throughout a simulation.

$$U_{bonded} = U_{bond} + U_{angle} + U_{torsion}$$

- **Bond Stretching:** Bond stretching is often modelled using harmonic potentials, ensuring atoms remain near their equilibrium bond lengths unless perturbed by thermal fluctuations or external forces.

$$U_{bond} = \frac{1}{2} k_b (r - r_0)^2$$

- **Angle Bending:** Bond angles also fluctuate around ideal geometries. Angle bending potentials restrict distortions that would otherwise destabilize molecular frameworks.

$$U_{angle} = \frac{1}{2} k_\theta (\theta - \theta_0)^2$$

- **Torsional (Dihedral) Rotations:** Torsional potentials describe how molecules rotate around bonds. These are particularly important in proteins, polymers, and organic molecules where conformational flexibility dictates structure and function.

$$U_{torsion} = k_\phi [1 + \cos(n\phi - \delta)]$$

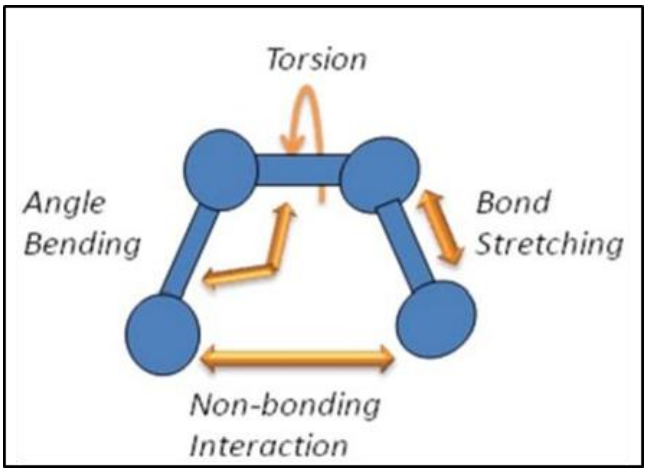

Figure 2 Chemical bonds (bond stretching, angle bending, torsion) and non-bonding interaction

- **Hydrogen Bonding:** Hydrogen bonding may be included explicitly or implicitly depending on the force field. While some models have specific terms for hydrogen bonding, many modern force fields capture its effects through a combination of electrostatics and van der Waals interactions.

$$U_{HB}(r) = Ar^{-12} - Br^{-10}$$

3. Lennard-Jones potential

The Lennard-Jones (LJ) potential is one of the foundational mathematical models used to describe van der Waals interactions in classical Molecular Dynamics simulations. It captures the essential balance between short-range repulsion arising from electron cloud overlap and intermediate-range attraction arising from dispersion (London) forces. Despite its simplicity,

the LJ potential reproduces fundamental features of atomic interactions and remains widely used for liquids, noble gases, soft matter systems, and as the non-bonded component of many biomolecular force fields.

Mathematically, the LJ potential is expressed as:

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

$\boldsymbol{r}$ is the interatomic distance,

$\boldsymbol{\varepsilon}$ is the depth of the potential well (interaction strength),

$\boldsymbol{\sigma}$ is the finite distance at which [potential is zero representing an effective particle diameter.

The first term, $\left(\frac{\boldsymbol{\sigma}}{\boldsymbol{r}}\right)^{12}$, represents steep repulsion due to Pauli exclusion, while the second term, $\left(\frac{\boldsymbol{\sigma^6}}{\boldsymbol{r}}\right)$ models attractive dispersion forces. The potential reaches its minimum value at:

$$r_{min} = 2^{1/6}\sigma \quad \& \quad U(r_{min}) = -\varepsilon$$

The corresponding force between two atoms is obtained by differentiating the potential:

$$F_{LJ}(r) = -\frac{dU}{dr} = 24\varepsilon\left[\frac{2\sigma^{12}}{r^{13}} - \frac{\sigma^{6}}{r^{7}}\right]$$

This force naturally transitions from strongly repulsive at short distances to weakly attractive at intermediate distances, stabilizing intermolecular spacing.

In practical MD simulations, LJ interactions are evaluated only up to a cutoff distance (r_c) (typically 8-12 Å) to reduce computational effort. Because the LJ potential does not naturally become zero at (r_c), many implementations apply shifting or switching functions to maintain energy and force continuity. Analytical tail corrections may be applied for energy and pressure when simulating homogeneous fluids.

When simulating mixtures or multi-species systems, the LJ parameters for unlike pairs are computed using combining rules. The most common Lorentz-Berthelot rules are:

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}, \ \varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}$$

The LJ potential is frequently paired with electrostatic terms to form the complete non-bonded interaction model used in large biomolecules and materials. Its mathematical simplicity, physical realism, and computational efficiency make it central to the development and application of classical molecular simulations.

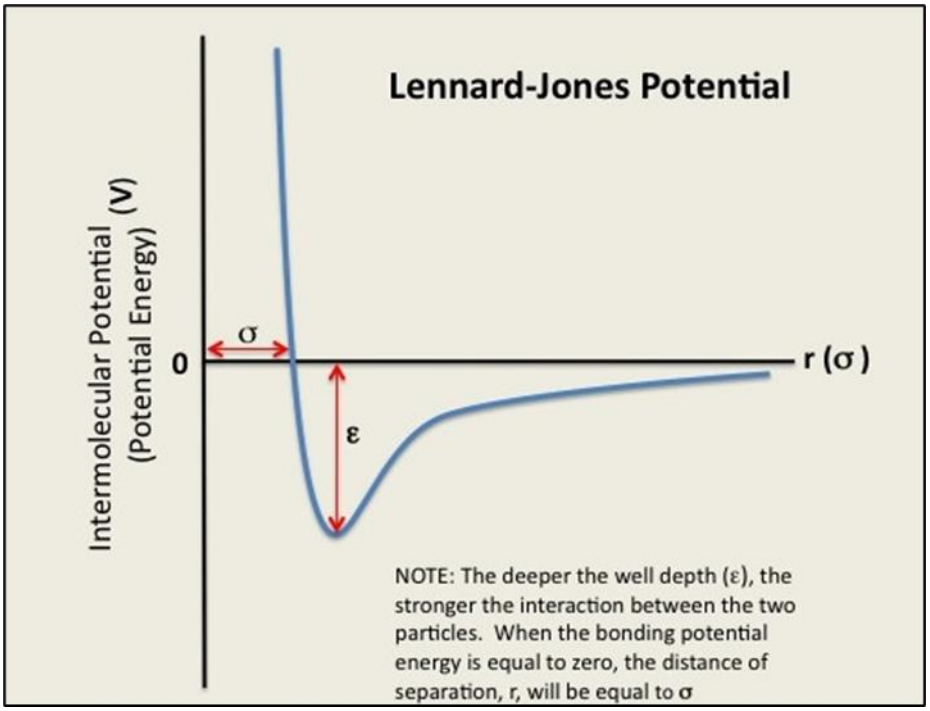

Figure 3 Lennard-Jones potential showing well depth (ε) and characteristic distance (σ)

4. Methodology

A variety of software tools were used to carry out the programming and Molecular Dynamics (MD) simulations. The main simulations were done with MD engines like GROMACS, NAMD, CHARMM, AMBER, Open Babel, VMD, and UCSF Chimera. While choosing software offers some flexibility, it is important to remember that different engines use different Force Fields. For preparing and analyzing simulations, the workflow depended on programs that come with these MD engines, along with the MD Analysis package for specific needs. In addition, Bash and Python scripting skills were used for file manipulation, data formatting, and post-processing tasks.

To see the simulation coordinate trajectories, software like VMD and PyMOL was used. VMD is especially noted for being free and working with trajectory formats from most MD engines. Finally, plotting tools like gnuplot, xmgrace, qtgrace, R, and Excel were used to create graphical representations of the analysis data.

Table 1

Application of different force fields

	Target application
DL_POLY	The multi-purpose package is used for MD modelling a wide variety of molecular systems - from simple atomic fragments to ionic structures,

	polymers and biochemical macromolecules.
AMBER	Simulation of peptide, protein, nucleic acid, and small organic molecules to facilitate simulations of drugs and small molecule ligands in conjunction with biomolecules, carbohydrates, lipids
CHARMM	Simulation of peptides, proteins, prosthetic groups, small molecule ligands, nucleic acids, lipids, and carbohydrates occurs in solution, crystals, and membrane environments. CHARMM also finds broad applications for inorganic materials, including applications in materials design.
NAMD	This package is designed for high-performance simulation of large biomolecular systems.

Initial (Cartesian) coordinates for proteins can often be obtained from the Protein Data Bank (PDB) in PDB file format. These should be checked for missing or incomplete
residues, poorly resolved electron density, mutations introduced to aid crystallisation, etc. Missing residues can be built using software such as Modeller or DeepView.
Software such as VMD can generate chemically plausible coordinates for biopolymers.
Modeller can build structures based on homology; myriad homology modeling web servers exist. Coordinates for small molecules may be available from the Cambridge Structural Database or generated using software such as Avogadro.
Coordinates not derived from experimental data should ideally be optimised using quantum chemical calculations or extensive MD simulations.
Pre-equilibrated boxes of solvent coordinates are available for common solvents such as water

Force field files are essential for Molecular Dynamics (MD) simulations. They list parameter values and specify how these values apply to atom types and bonded interactions. Each MD software package requires these files to be in a specific format and usually comes with libraries for common force fields. It is important to keep things consistent; parameter values cannot be exchanged between force fields because they are set using different strategies and terms. Therefore, all molecules in a single simulation must use the same or a fully compatible force field to ensure accuracy.

When constructing molecules, "building blocks" (fragments or whole molecules) provide the needed parameters. For polymers like proteins, preparation programs within the MD software

link these amino acid building blocks to create the overall molecular structure. If a specific building block is not available, the molecule must be parameterized, either manually or with automated software. Common tools for this include ATB (for GROMOS), CherryPicker, CGenFF (for CHARMM), Antechamber (for AMBER/GAFF), and LigParGen (for OPLS). Additionally, choosing the environment is crucial since each force field only works with certain solvent models.

Molecular Dynamics run files are specific to each package and act as the blueprint for the simulation. They include all necessary algorithms and parameter values. A crucial first step is energy minimization. This step relaxes the structure and removes steric clashes using standard methods like steepest descent or conjugate-gradient refinement. Important configuration settings for this phase include convergence criteria, the maximum number of minimization steps, and the frequency of data output. Additionally, initialization and heating phases, usually done in the NVT ensemble, require clear definitions for constraint algorithms, cutoff distances for non-bonded interactions, and the method for handling long-range electrostatic interactions.

For specific studies of chemical and biochemical systems, we used the DL_POLY computer code. Developed at Daresbury Laboratories by Bill Smith's molecular modeling group, this software runs on an architecture with three input files-CONFIG, CONTROL, and FIELD-and generates three output files: OUTPUT, REVCON, and HISTORY. The CONFIG file sets up the initial state and includes boundary conditions, 3-dimensional coordinates, velocities, and interatomic forces. This file must be consistent with the FIELD file, which describes atomic structures, masses, charges, and interaction potentials. The CONTROL file defines the simulation environment and specifies parameters like temperature, pressure, integration steps, and specific methods used.

The main benefit of DL_POLY is its versatility. It allows the study of dynamic and structural properties across a wide range of molecular systems. It can simulate simple atomic systems and mixtures (e.g. Ne, Ar, Kr, etc.), unpolarizable point ions (e.g. NaCl, KCl, etc.), and more complex polarizable ions (e.g. MgO, H_2O etc.) or rigid molecules (CCl_4, SF_6, Benzene, etc.). Its usefulness also extends to rigid molecular ions (e.g. KNO_3, $(NH_4)_2SO_4$, etc.), polymers with rigid bonds (e.g. C_nH_{2n+2}), and complex biological macromolecules, including proteins. This broad capability makes it a useful tool for materials ranging from basic ionic structures to complex biological assemblies.

5. Application of MD and Continuum Modelling in Battery Research

5.1 Atomistic-Scale Analysis Through Molecular Dynamics (MD)

As part of my work on battery materials, I employ molecular dynamics (MD) simulations to investigate ion transport and interfacial behaviour at the atomic scale. MD provides a physics-based framework for modelling the motion of atoms and molecules using Newton's equations of motion,

$$m_i \frac{d^2 r_i}{dt^2} = -\nabla_i U(r_1, r_2, \dots, r_N)$$

where (U) is the potential energy surface constructed from van der Waals, electrostatic, and bonded interactions. By parameterizing this potential using appropriate force fields, I can simulate the dynamical evolution of electrolyte molecules, lithium ions, and solvent structures under realistic temperature and pressure conditions. These simulations allow me to quantify key microscopic properties such as ionic diffusion coefficients, solvation structures, ion-pair formation tendencies, and local structural rearrangements of the electrolyte environment.

Transport parameters extracted from MD play a crucial role in understanding electrolyte performance. For instance, the self-diffusion coefficient of Li^+ is evaluated from the Einstein relation,

$$D = \frac{1}{6} \frac{d}{dt} \langle |r(t) - r(0)|^2 \rangle$$

which provides a direct connection between atomic trajectories and macroscopic transport behaviour. Similarly, radial distribution functions (RDFs) computed from MD trajectories help identify preferred coordination environments and quantify the stability of solvation shells. These atomistic insights form the foundation for interpreting how molecular-scale interactions influence the conductivity, viscosity, and thermal response of electrolyte formulations that I study experimentally.

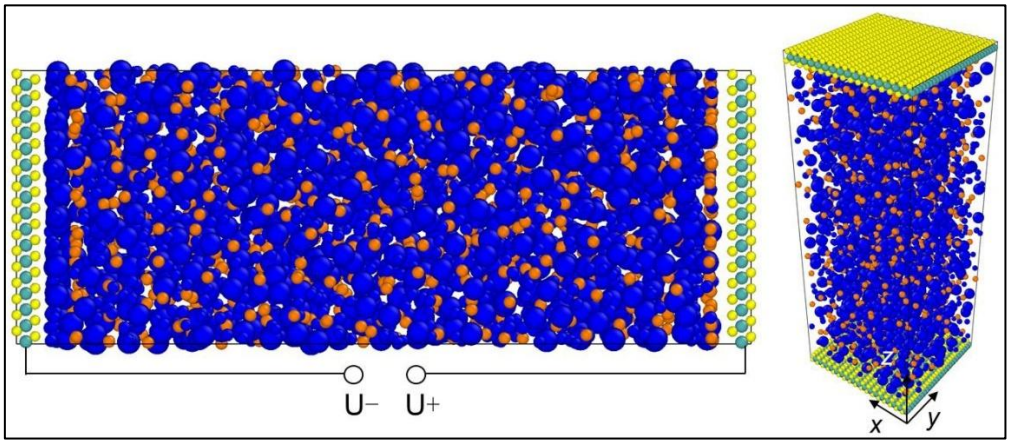

Figure 4 MD simulation of [BMI^+][PF_6^-] electrolyte at a MoS_2 electrode. Cations (blue), anions (orange); Mo (green), S (yellow).

5.2 Continuum-Scale Modelling Through COMSOL Multiphysics

To translate atomistic behaviour into cell-level electrochemical predictions, I integrate my MD results into continuum-scale models built using COMSOL Multiphysics. COMSOL provides a physics-driven platform for simulating concentration gradients, charge-transfer processes, and potential distributions within battery cells. The "Transport of Diluted Species" and "Electrochemistry" modules allow me to incorporate MD-derived parameters such as diffusion coefficients, transference numbers, and solvation-dependent mobilities into the governing transport equations.

At this scale, ionic transport is described using the Nernst-Planck equation,

$$J_i = -D_i \nabla c_i - z_i u_i F c_i \nabla \phi$$

where (D_i) is the diffusion coefficient (extracted from MD), (u_i) is ionic mobility, and (ϕ) is the electric potential. This formulation accounts for both concentration-driven diffusion and field-driven migration, enabling realistic modelling of electrolyte behaviour under operating currents.

Electrode processes are captured by the Butler-Volmer equation,

$$i = i_0 \left[\exp\left(\frac{\alpha_a F \eta}{RT}\right) - \exp\left(-\frac{\alpha_c F \eta}{RT}\right) \right]$$

which relates local overpotential (η) to interfacial reaction kinetics. Parameters such as activation energies or adsorption energies-estimated from MD or hybrid MD-QM calculations-

can be incorporated here to represent how interfacial molecular structure influences charge-transfer rates. Through these equations, COMSOL allows me to simulate cell-level phenomena such as electrolyte depletion at high rates, potential drop across electrodes, SEI-related resistance evolution, and mass-transport limitations.

5.3 Multiscale Integration and Impact on My Battery Research

The integration of MD and COMSOL forms a multiscale pipeline that enhances my ability to understand, predict, and optimize battery behaviour. MD provides molecular-level insight into ion-solvent interactions, solvation energy changes, and interfacial structure evolution, while COMSOL translates these microscopic features into macroscopic performance indicators such as overpotential, ionic conductivity, and rate capability. This linkage ensures that continuum-level simulations do not rely on empirical guesses but are grounded in atomistic data that reflect the actual molecular environment of the battery system.

This multiscale approach is particularly valuable for interpreting discrepancies between experimental observations and theoretical expectations. For example, if an electrolyte shows high ionic conductivity experimentally but performs poorly at high rates, MD can reveal whether strong ion-solvent binding or transient aggregates hinder mobility. COMSOL then shows how these microscopic features manifest as concentration gradients, voltage losses, or limited diffusion at the electrode surface. Together, the two techniques enable a more mechanistic understanding of electrolyte behaviour and guide the optimization of solvent systems, salt concentrations, and interfacial chemistries. By incorporating both atomistic and continuum simulations alongside my lab-scale experimental work, I can evaluate electrolyte performance from first principles, predict behaviour in untested conditions, and design improved formulations with higher ionic transport efficiency and more stable interfacial behaviour. This integrated computational direction significantly strengthens the scientific depth and predictive capability of my ongoing battery research.

6. Conclusion

Taken together, the methodological integration of molecular dynamics simulations with continuum-scale electrochemical modelling constitutes a comprehensive and scientifically rigorous multiscale framework that significantly strengthens the depth, reliability, and predictive capability of my ongoing research on battery materials. At the atomistic level, molecular dynamics provides a detailed mechanistic perspective on the structural and

dynamical behaviour of electrolyte species, allowing for the direct resolution of ion trajectories, solvation-shell organization, and interfacial interactions through the numerical solution of Newton's equations of motion and the computation of key microscopic descriptors such as diffusion coefficients, mean-squared displacements, and radial distribution functions. These outputs form a quantitatively robust representation of the molecular environment that cannot be accessed through experimental measurements alone. The derived transport and interaction parameters, grounded in fundamental interatomic potentials, serve as essential inputs for continuum-scale models built in COMSOL Multiphysics, where species transport and electrochemical kinetics are governed by formal transport and reaction equations-most notably the Nernst-Planck formulation for ionic fluxes and the Butler-Volmer relation for charge-transfer dynamics. Incorporating MD-derived values into these models ensures that the continuum-level simulations reflect the true molecular physics of the system rather than relying on empirical fitting or assumed literature constants. This multiscale coupling thereby establishes a direct and scientifically defensible link between molecular interactions and device-level phenomena, enabling the prediction and interpretation of concentration gradients, electrical potential distributions, interfacial reaction rates, and performance limitations under practically relevant operating conditions. Moreover, the integrated approach enhances the interpretive resolution of my experimental findings by providing atomistically informed explanations for macroscopic behaviours such as rate performance, kinetic overpotentials, electrolyte depletion, and SEI-related impedance growth. Beyond interpretation, this combined modelling framework facilitates rational materials optimization by enabling the systematic evaluation of electrolyte compositions, solvation environments, and electrode surface chemistries prior to experimental synthesis. Overall, the synergy between MD and COMSOL establishes a robust, hierarchical modelling strategy that unifies fundamental molecular-scale physics with applied electrochemical engineering, thereby providing a strong theoretical and computational foundation that supports the continued advancement of my research on high-performance battery systems.

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