

Mathematical Modeling in Nanotechnology- An Overview

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Abstract

Nanotechnology is a rapidly evolving field that focuses on the manipulation and control of materials at the nanoscale. The complexity and intricacy of nanoscale systems often require sophisticated mathematical models to understand and predict their behavior. Mathematical modeling plays a crucial role in elucidating the fundamental principles governing various nanoscale phenomena and enables the design and optimization of nanodevices and processes. This paper provides a comprehensive review of mathematical modeling techniques and their applications in nanotechnology. It explores the theoretical foundations of mathematical modeling in nanoscale systems and discusses its wide-ranging applications, including nanomaterials synthesis, nanoparticle characterization, nanofluidics, nanoelectronics, and nanomedicine. Furthermore, the paper highlights the challenges and limitations associated with modeling at the nanoscale and discuss future prospects and directions for advancements in this interdisciplinary field.

1. Introduction

One of the most active research fields in the scientific community today is nanotechnology. Physics, chemistry, biology, and engineering are just a few of the sciences that are combined in the multidisciplinary field of nanotechnology study. Additionally, by developing novel applications in this field, mathematical modeling might help us better understand how nanostructured materials behave in various situations. Since last ten years, almost 180 articles have been published and more than 7000 citations have been received. **Figure 1 (a)** and **figure 1 (b)** shows the graphs of year wise article published and total year wise citations received. The data has been taken from **Scopus database**.

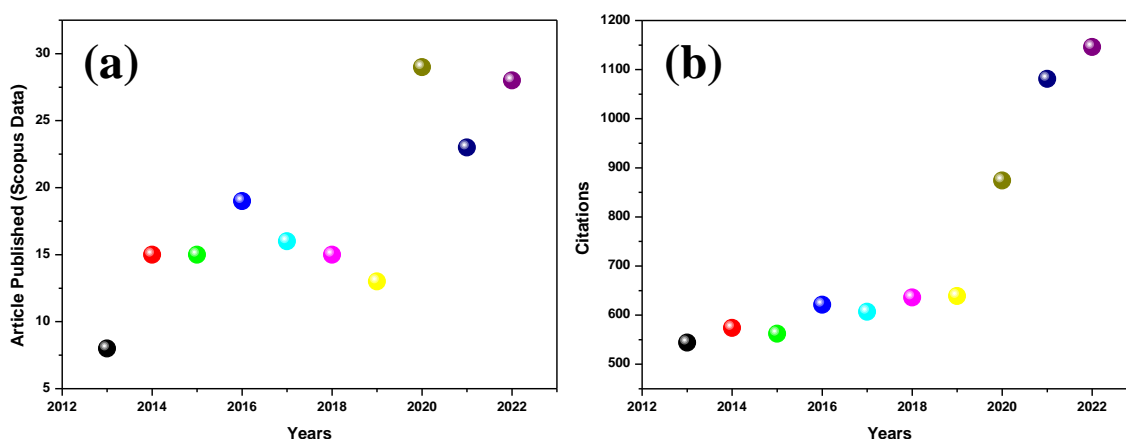


Figure 1: Figure 1(a) Total year wise article published, and (b) Total year wise citations received (Source: https://scopus.com/cto2/main.uri?origin=resultslist&stateKey=CTOF_1671767286#citationOverviewTable)

1.1. Overview of nanotechnology and its significance

Nanotechnology is a multidisciplinary field that focuses on the understanding, manipulation, and control of matter at the nanoscale, typically ranging from 1 to 100 nanometers (nm). At this scale, materials exhibit unique properties and behaviors that are distinct from their bulk counterparts. These properties arise due to the increased surface-to-volume ratio, quantum effects, and enhanced surface reactivity.

The significance of nanotechnology lies in its potential to revolutionize various industries and fields, offering unprecedented opportunities for advancements in technology, medicine, energy, materials science, and environmental sustainability [1]. Some key areas where nanotechnology has made significant contributions include:

Electronics and Computing: Nanotechnology has enabled the miniaturization of electronic components, leading to faster and more efficient electronic devices. Nanoscale transistors, nanowires, and quantum dots have paved the way for advancements in computing power, memory storage, and sensor technology [2-4].

Aerospace industries: Nanotechnology has the promising applications in aerospace engineering. Carbon nanotubes, graphene, polymer nanocomposites, and nanocomposite based coatings can improve the thermal, electrical, and mechanical performance of the aerospace structures. Similarly, integration of highly sensitive nanosensors and flexible material based sensors and nanoelectronics into the aerospace systems such as navigation, communication and control can enhance the accuracy, functionality, and sensitivity of aerospace systems. Such nanosensors can enable more precise and strong measurements of several parameters such as pressure, strain, temperature, magnetic field, and acceleration. Such sensors can also monitor the different kinds of pollutant and pathogens. Nanosensors and nanoelectronics can also enable the networked and wireless systems to communicate with each other and with ground station and satellites [5-7].

Medicine and Healthcare: Nanotechnology has transformed the field of medicine, enabling targeted drug delivery, early disease detection, cancer therapy, antiviral therapeutic agents, and innovative therapies [8, 9]. Nanoparticles, nanocarriers, and nanosensors can be designed to interact specifically with biological systems, enhancing drug efficacy and reducing side effects [8, 9]. In medical field, the toxicity of the nanomaterials is also an issue. Therefore, the understanding and the mechanism of the toxicity of nanomaterials is necessary. In this regard, Gupta et al [10] has discussed about the nanoparticles, their toxic behaviour and the underlying mechanism of toxicity of nanomaterials in biological fields.

Energy and Environment: Nanomaterials are being explored for energy storage, conversion, and conservation. Nanoscale catalysts have improved the efficiency of chemical reactions, while nanocomposites and nanofabrication techniques have enhanced the performance of solar cells and batteries. Nanotechnology also offers potential solutions for environmental remediation and water purification. Porous carbon materials and 2-dimensional graphene is widely used in water purification. Bhatnagar et al has reported the modified activated carbon by using appropriate precursor and also the modified treatment method for removal of specific pollutants [11]. Sweetman et al [12] has shown the use of carbon based materials such as activated carbon, graphene and carbon nanotubes and their composites for water purification. Recent advancement in water purification system using carbon based materials and their applicability in point-of-use water purification systems has also been discussed (see figure 2).

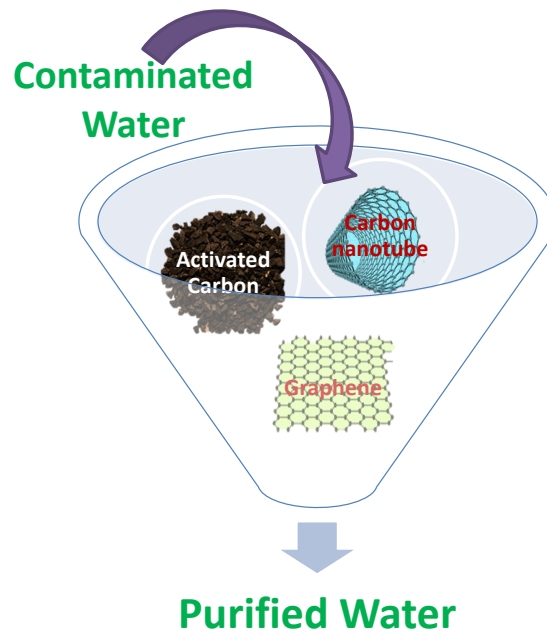


Figure 2: Carbon based materials for water purification

At present, society is suffering from the need of highly efficient energy systems such as energy generation, energy storage, energy conversion, saving and transmission for day-to-day life. In this field, multifunctional nanomaterials can play an important role in such applications due to their extraordinary electrical, mechanical, thermal, optical, catalytic etc. In this nanoscale range, piezoelectric, catalytic, triboelectric, and thermoelectric materials play an important role in energy applications [13].

Materials Science and Engineering: Due to the high surface-to-volume ratio, nanomaterials exhibit exceptional mechanical, thermal, optical, electrical properties, and chemical stability. These materials, such as carbon nanotubes, graphene, and nanocomposites, have revolutionized the development of lightweight and high-strength materials for various applications, including aerospace, construction, EMI shielding, strain sensing, and consumer electronics. Carbon nanotube and graphene reinforced nanocomposites contribute to further enhance the strength and shock absorption of frames, cranks, handlebars, front forks, etc. Usually, in such applications, MWCNT are used expecting the increase in compressive strength, and carbon fiber contributes to the tensile strength [14-16]. The attractive electrical and mechanical properties of these composites also find applications in electrochemical applications such as supercapacitors and other energy storage devices [17].

Environmental Sensing: Nanosensors and nanodevices are capable of detecting and monitoring environmental pollutants, toxins, and pathogens with high sensitivity and selectivity. This enables real-time monitoring of air and water quality, food safety, and early warning systems for potential hazards [18, 19].

Agriculture and Food Technology: Nanotechnology holds promise for improving crop yields, nutrient delivery systems, and food packaging. Nanoscale formulations can enhance the efficiency of fertilizers and pesticides, while nanostructured packaging materials can improve food safety and preservation [20-23].

The significance of nanotechnology arises from its ability to manipulate matter at the atomic and molecular levels, leading to precise control over material properties and functionalities. This level of control offers unprecedented opportunities to overcome

existing technological limitations, develop novel materials and devices, and address pressing societal challenges. Furthermore, nanotechnology has the potential to drive economic growth, create new industries and job opportunities, and contribute to sustainable development.

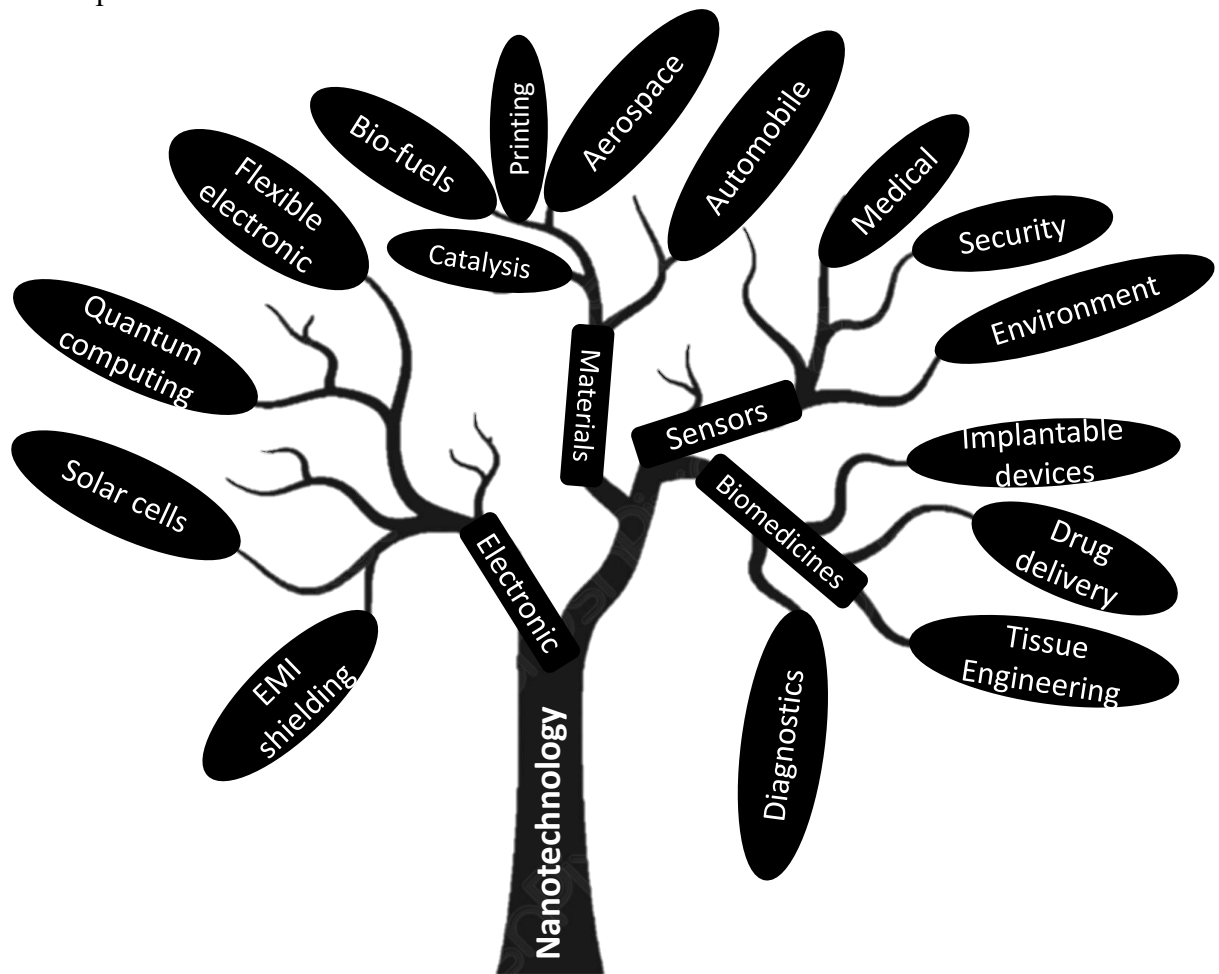


Figure 3: Various applications of nanotechnology different fields

However, as nanotechnology progresses, it is essential to address potential ethical, environmental, and safety concerns associated with the release and exposure to nanomaterials. Robust regulations, responsible research practices, and risk assessment frameworks are crucial to ensure the safe and responsible development and deployment of nanotechnology.

In summary, nanotechnology represents a transformative field that has the potential to reshape various industries and positively impact society. Its significance lies in its ability to harness the unique properties of nanoscale materials and devices, leading to innovations in electronics, medicine, energy, materials science, and environmental sustainability. By combining scientific advancements with responsible practices, nanotechnology holds the key to addressing critical challenges and improving the quality of life for people around the world. **Figure 3** shows the various applications of nanotechnology in diverse field of science and technology, and biomedical science [24].

1.2.Role of mathematical modeling in nanoscale systems

The role of mathematical modeling in nanoscale systems is paramount, as it provides a powerful framework for understanding, predicting, and optimizing the behavior and properties of nanomaterials, nanodevices, and nanoscale processes. Mathematical modeling allows researchers to gain insights into complex phenomena that are difficult to observe directly or are cost-prohibitive to study experimentally. It serves as a bridge between theoretical understanding and experimental observations, enabling scientists to explore and design nanoscale systems in a systematic and efficient manner. Here are some key roles of mathematical modeling in nanoscale systems:

Understanding Nanoscale Phenomena: Mathematical models provide a quantitative description of the underlying physical, chemical, and biological processes that occur at the nanoscale. By formulating mathematical equations based on fundamental principles, researchers can elucidate the mechanisms governing nanoscale phenomena and gain a deeper understanding of the behavior of nanoscale systems.

Predicting and Optimizing Nanoscale Behavior: Mathematical models allow for the prediction of nanoscale behavior under different conditions. By simulating and analyzing the behavior of nanoscale systems using mathematical equations and computational algorithms, researchers can optimize parameters and design principles to achieve desired functionalities. This helps in guiding experimental efforts and reducing trial-and-error approaches.

Exploring Multiscale Interactions: Nanoscale systems often involve interactions and dynamics at multiple length and time scales. Mathematical modeling facilitates the integration of different scales, allowing researchers to investigate how phenomena at one scale influence and propagate to others. Multiscale modeling approaches enable the study of complex nanoscale systems that exhibit emergent properties arising from the interactions of individual components.

Designing Nanomaterials and Nanodevices: Mathematical modeling plays a crucial role in the design and optimization of nanomaterials and nanoscale devices. By modeling the structural, electronic, and optical properties of nanomaterials, researchers can tailor their characteristics to achieve specific functionalities. Similarly, mathematical models assist in the design of nanoscale devices, such as sensors, actuators, and electronic circuits, optimizing their performance based on desired specifications [25].

Overcoming Experimental Limitations: Experiments at the nanoscale can be challenging due to limitations in observation techniques, time scales, and sample availability. Mathematical modeling serves as a complementary tool to experimental investigations, providing insights into phenomena that are difficult to measure directly. Models can help extrapolate experimental data, predict behavior beyond the experimental regime, and guide the design of new experiments.

Guiding Nanoscale Manufacturing and Processes: Mathematical models aid in optimizing nanoscale fabrication techniques and manufacturing processes. By simulating and analyzing the relevant physical and chemical processes involved in nanoscale synthesis, assembly, and manipulation, researchers can improve process efficiency, reduce costs, and ensure product quality. This helps in scaling up nanoscale processes for practical applications.

Exploring New Possibilities and Innovations: Mathematical modeling in nanoscale systems enables researchers to explore new concepts and push the boundaries of what is possible. It allows for the investigation of hypothetical scenarios, the discovery of new

phenomena, and the identification of design principles that lead to novel functionalities. Mathematical modeling provides a creative space for exploring innovative ideas and driving technological advancements.

2. Mathematical Modeling Fundamentals

2.1. Principles and methodologies of mathematical modelling

Principles and methodologies of mathematical modeling provide a systematic framework for representing and analyzing complex systems using mathematical equations and computational algorithms. These principles guide the process of formulating mathematical models, validating them against experimental data, and using them to gain insights into the behavior of the systems being studied. Here are key principles and methodologies of mathematical modeling:

Conceptualization: The first step in mathematical modeling is to conceptualize the system of interest and identify the key components, variables, and interactions that govern its behavior. This involves understanding the underlying physical, chemical, or biological principles and simplifying the system into manageable components.

Formulation: Mathematical models are formulated by translating the conceptualized system into a set of mathematical equations or computational algorithms. These equations describe the relationships between the variables and parameters of the system, capturing the cause-and-effect relationships and dynamics.

a. Deterministic Modeling: Deterministic modeling assumes that the system behavior is entirely determined by the given inputs and parameters. It uses ordinary differential equations (ODEs) or partial differential equations (PDEs) to describe the system's evolution over time or space.

b. Stochastic Modeling: Stochastic modeling considers random fluctuations and uncertainties in the system. It employs probabilistic models, such as stochastic differential equations (SDEs) or Monte Carlo simulations, to account for the inherent randomness and variability in the system's behavior.

Model Calibration and Validation: Once the mathematical model is formulated, it needs to be calibrated and validated against experimental data or known reference cases. Model calibration involves estimating the model parameters to best fit the observed data, while model validation assesses the model's accuracy and predictive capability against independent datasets. Iterative refinement of the model may be necessary to achieve a good fit and predictive accuracy.

Simulation and Analysis: Once the model is calibrated and validated, it can be used to simulate the behavior of the system under different conditions or scenarios. Numerical methods, such as finite difference methods, finite element methods, or numerical optimization techniques, are employed to solve the mathematical equations or perform simulations. The results are analyzed to gain insights into the system's behavior, identify patterns, and make predictions.

Sensitivity Analysis and Parameter Estimation: Sensitivity analysis examines the impact of variations in model inputs and parameters on the model outputs. It helps identify the most influential factors and assesses the robustness of the model predictions. Parameter estimation involves estimating unknown or uncertain model parameters using optimization

techniques, statistical methods, or data assimilation techniques to improve the model's accuracy.

Model Validation and Verification: Model validation involves comparing the model predictions with new experimental data or independent datasets that were not used during model calibration. Model verification ensures that the mathematical model has been implemented correctly by comparing the model's implementation with known analytical solutions or benchmark cases, if available.

Model Complexity and Trade-offs: Mathematical models can range from simple analytical expressions to complex numerical simulations. Model complexity should be chosen based on the trade-off between accuracy and computational cost. Simpler models are computationally efficient but may overlook important details, while more complex models capture finer nuances but require more computational resources.

Iterative Refinement and Model Updating: Mathematical models are not static; they evolve and improve over time. As new data and insights become available, models can be refined, updated, or extended to incorporate additional features or phenomena. The iterative process of refining the model based on new information helps improve its accuracy and predictive capability.

These principles and methodologies provide a systematic approach for developing mathematical models that capture the essential features of complex systems. They enable scientists and researchers to gain deeper insights into the behavior of systems, make predictions, optimize designs, and guide experimental investigations. However, it is important to recognize the limitations of mathematical models and their assumptions, as well as to integrate them with experimental data and empirical observations for a comprehensive understanding of the system under study.

2.2. Deterministic and stochastic modeling approaches

Deterministic and stochastic modeling approaches are two distinct methodologies used in mathematical modeling to capture different aspects of system behavior and uncertainty.

Deterministic Modeling:

Deterministic modeling assumes that the system behavior is completely determined by the given inputs and parameters, without accounting for random fluctuations. It aims to describe the system's evolution over time or space using deterministic equations, typically in the form of ordinary differential equations (ODEs) or partial differential equations (PDEs).

In deterministic modeling:

- The state variables of the system are assumed to have precise, well-defined values at any given time.
- The model produces a single, definite trajectory of the system's behavior for a given set of initial conditions and inputs.
- Deterministic models are often used when the system's behavior is well understood and predictable, without significant random or stochastic influences.
- Deterministic modeling is widely employed in various fields, including physics, engineering, and biology, where the underlying dynamics can be accurately represented by deterministic equations. It allows for the analysis of system stability, equilibrium points, and the exploration of different parameter regimes to understand the system's behavior.

Stochastic Modeling:

Stochastic modeling incorporates randomness and uncertainty into the system's behavior, acknowledging that certain aspects of the system are subject to random fluctuations or influences that cannot be precisely predicted. It employs probabilistic models and statistical methods to capture the variability and inherent randomness in the system.

In stochastic modeling:

- The state variables of the system are represented as random variables or stochastic processes, characterized by probability distributions.
- The model generates a range of possible outcomes or trajectories, instead of a single definitive trajectory, reflecting the inherent uncertainty in the system.
- Stochastic models are often used when the system involves inherent variability, noise, or random events that significantly impact its behavior.
- Stochastic modeling allows for the analysis of statistical properties, such as mean, variance, and higher-order moments of the system's behavior. It enables the assessment of system reliability, estimation of probabilities, and investigation of rare events. Stochastic modeling techniques include stochastic differential equations (SDEs), Monte Carlo simulations, and Markov chains.
- Stochastic modeling finds applications in various fields, such as finance, ecology, genetics, and queuing theory, where uncertainty and randomness play significant roles. It is particularly useful when the system involves fluctuations, external disturbances, or limited knowledge about precise system parameters.

In many cases, a combination of deterministic and stochastic modeling approaches is employed, where deterministic models provide the overall system behavior, and stochastic models capture the random fluctuations or uncertainties around the deterministic predictions. This hybrid approach allows for a more comprehensive understanding of the system's behavior, incorporating both deterministic trends and stochastic influences.

The choice between deterministic and stochastic modeling approaches depends on the nature of the system, the available data, and the research objectives. Understanding the underlying dynamics and sources of uncertainty is essential for selecting the appropriate modeling methodology to accurately represent and analyze the system.

2.3. Multi-scale modeling techniques

Multi-scale modeling techniques are employed in mathematical modeling to capture phenomena that occur at different length scales within a system. These techniques allow researchers to bridge the gap between the behavior of individual components and the collective behavior of the system as a whole. Multi-scale modeling is particularly useful when studying complex systems that exhibit emergent properties arising from interactions across multiple scales. Here are some commonly used multi-scale modeling techniques:

Hierarchical Modeling:

Hierarchical modeling involves constructing a hierarchy of models, where each level of the hierarchy represents a different scale of the system. The models at different scales are interconnected, with information and parameters flowing between them. This approach allows for the incorporation of detailed, fine-scale models within a larger, coarse-scale

model. It enables the study of how phenomena at one scale influence or emerge from the interactions at other scales.

Continuum Modeling:

Continuum modeling treats the system as a continuous medium, assuming that the properties and behavior can be described by continuous fields, such as temperature, density, or concentration. Continuum models, such as partial differential equations (PDEs), capture the macroscopic behavior of the system and are typically valid at larger length scales. These models provide averaged descriptions of the system, ignoring fine-scale details and heterogeneities.

Molecular Dynamics (MD) Simulations:

Molecular Dynamics simulations model systems at the atomic or molecular level, tracking the individual particles' positions, velocities, and interactions over time. MD simulations are based on Newtonian mechanics and interatomic potential energy functions. They provide detailed information about the system's dynamics, structure, and properties at the atomic scale. MD simulations are particularly useful for studying materials, biomolecules, and chemical reactions at the nanoscale.

Coarse-graining:

Coarse-graining is a technique that simplifies a system by reducing the number of degrees of freedom while preserving essential features. It involves grouping multiple interacting components into coarse-grained particles or regions. Coarse-grained models effectively represent the collective behavior of the system and are computationally more efficient than atomistic models. The parameters of coarse-grained models are often derived from more detailed, atomistic simulations or experimental data.

Agent-based Modeling:

Agent-based modeling simulates the behavior of individual agents or entities in a system and their interactions. Each agent follows specified rules and can have its own internal state and behavior. Agent-based models capture the emergent behavior arising from the interactions of multiple agents. They are useful for studying complex systems, such as biological systems, social dynamics, and traffic flow, where individual-level interactions lead to collective behavior.

Hybrid Modeling:

Hybrid modeling combines different modeling techniques, such as continuum modeling, discrete particle simulations, or network modeling, to capture different aspects of a system at different scales. It allows for the integration of multiple modeling approaches to address specific features or phenomena of interest. Hybrid models often involve coupling or exchanging information between different modeling frameworks to capture the interactions and dynamics across scales.

The choice of multi-scale modeling technique depends on the specific characteristics of the system, the phenomena of interest, and the available computational resources. Multi-scale modeling provides a powerful approach to study and understand complex systems, capturing the interactions and emergent behavior that arise from interactions at multiple scales. It enables researchers to gain insights into system behavior from the microscopic to macroscopic levels, contributing to a more comprehensive understanding of the system as a whole.

3. Modeling Nanomaterials Synthesis

3.1. Kinetic models for nanoparticle growth and assembly

Kinetic models play a crucial role in understanding the growth and assembly processes of nanoparticles. These models describe the evolution of nanoparticle size, shape, and composition over time, taking into account the underlying physical and chemical mechanisms involved. By capturing the kinetics of nanoparticle growth and assembly, these models provide insights into the factors influencing nanoparticle properties and enable the design and optimization of synthesis strategies. Here are some commonly used kinetic models for nanoparticle growth and assembly:

Nucleation and Growth Models:

Nucleation and growth models describe the formation of nanoparticles from precursor species through the nucleation of small clusters, followed by their subsequent growth. These models typically involve rate equations that track the concentration or number of clusters and monomers over time. The nucleation step considers factors such as supersaturation, temperature, and precursor concentration, while the growth step accounts for monomer attachment and surface diffusion processes.

Aggregation and Coalescence Models:

Aggregation and coalescence models focus on the assembly and merging of nanoparticles into larger structures. These models describe the collision, attachment, and rearrangement of nanoparticles, accounting for factors such as particle concentration, size distribution, and interparticle interactions. Models based on population balance equations or stochastic simulation algorithms capture the dynamics of aggregation and coalescence, allowing for the prediction of particle size distributions and morphology evolution.

Ostwald Ripening Models:

Ostwald ripening models explain the growth dynamics of nanoparticles by the gradual dissolution of smaller particles and the deposition of the dissolved material onto larger particles. These models consider the diffusion of material from smaller to larger particles driven by the concentration gradient. The rate of ripening is influenced by factors such as particle size distribution, solubility, and interfacial energy. Ostwald ripening models can predict changes in the size distribution and morphology of nanoparticles over time.

Kinetic Monte Carlo (KMC) Simulations:

Kinetic Monte Carlo simulations are computational modeling techniques used to study the dynamics of nanoparticle growth and assembly at the atomic or molecular level. KMC simulations track the individual particles' positions, velocities, and interactions over time, allowing for the exploration of various growth mechanisms and surface processes. By incorporating detailed atomic-scale information and reaction rates, KMC simulations provide insights into the kinetics and mechanisms of nanoparticle growth and assembly.

Discrete Element Modeling (DEM):

Discrete Element Modeling is a computational technique used to simulate the behavior of individual particles and their interactions in granular systems, including nanoparticle assemblies. DEM models consider the dynamics of particle collisions, adhesion, and interparticle forces. By accounting for factors such as particle size, shape, and surface properties, DEM simulations can predict the assembly behavior, packing structure, and mechanical properties of nanoparticle assemblies.

These kinetic models are continuously refined and adapted to capture the specific mechanisms and experimental conditions relevant to nanoparticle growth and assembly. They are often parameterized using experimental data and validated against experimental observations to ensure their accuracy and predictive capability. By employing these models, researchers can gain insights into the underlying mechanisms governing nanoparticle growth and assembly, optimize synthesis conditions, and tailor the properties of nanoparticles for various applications in fields such as materials science, catalysis, and nanomedicine.

3.2. Modeling self-assembly processes

Modeling self-assembly processes is essential for understanding and predicting the formation of ordered structures through the spontaneous organization of individual components. Self-assembly refers to the process by which these components interact and arrange themselves into well-defined patterns or structures without external intervention. Mathematical models play a crucial role in capturing the kinetics and thermodynamics of self-assembly, shedding light on the underlying mechanisms and enabling the design and control of self-assembled systems. Here are some common approaches to modeling self-assembly processes:

Statistical Mechanics Models:

Statistical mechanics models provide a theoretical framework for understanding self-assembly by describing the behavior of a system at the molecular or particle level. These models consider the interaction potentials between individual components, such as particles or molecules, and the thermal fluctuations of the system. Various techniques, such as Monte Carlo simulations or molecular dynamics simulations, can be used to explore the system's energy landscape, predict the equilibrium structures, and assess the kinetic pathways of self-assembly.

Lattice Models:

Lattice models simplify the self-assembly process by considering components as discrete entities occupying specific lattice sites. These models often assume simple interaction rules between neighboring components, allowing for efficient simulations and analysis. Lattice-based approaches, such as cellular automata or lattice Monte Carlo methods, facilitate the study of self-assembly phenomena, including crystallization, pattern formation, and phase transitions.

Coarse-grained Models:

Coarse-grained models provide a simplified representation of self-assembling systems by reducing the level of detail while retaining the essential interactions and structures. In these models, groups of particles or molecules are represented as effective entities, referred to as coarse-grained units. Coarse-grained models capture the mesoscale dynamics and structural features of self-assembled systems while reducing the computational complexity. These models are particularly useful for studying large-scale or long-time self-assembly processes.

Kinetic Monte Carlo (KMC) Simulations:

Kinetic Monte Carlo simulations model self-assembly processes by tracking the stochastic motion and interactions of individual components. These simulations consider the rates of particle attachment, detachment, and diffusion, as well as the local environment's effects. KMC simulations allow for the exploration of the time evolution and statistical properties

of self-assembled structures, enabling predictions of assembly kinetics and the influence of various factors on the resulting structures.

Reaction-Diffusion Models:

Reaction-diffusion models describe self-assembly processes as coupled chemical reactions and diffusive processes. These models account for the chemical reactions between components and their diffusion in the surrounding medium. Reaction-diffusion models can capture the emergence of spatial patterns and the formation of self-assembled structures, such as Turing patterns or wavefront propagation.

Computational Optimization and Genetic Algorithms:

Computational optimization techniques, including genetic algorithms and simulated annealing, can be employed to search for energetically favorable configurations or optimal parameters for self-assembly. These algorithms explore the parameter space and search for configurations that minimize the system's energy or maximize a desired property, leading to the identification of optimal self-assembled structures.

The choice of modeling approach depends on the specific self-assembly system, its complexity, and the level of detail required. These modeling approaches help researchers understand the driving forces, kinetics, and thermodynamics of self-assembly processes. They allow for the prediction of self-assembled structures, exploration of parameter space, and optimization of conditions to achieve desired structures and properties. Mathematical modeling of self-assembly processes is a valuable tool for designing and controlling self-assembled materials, nanoscale devices, and functional structures with applications in fields such as materials science, nanotechnology, and biophysics.

3.3. Computational modeling of nanoscale fabrication techniques

Computational modeling plays a crucial role in understanding and optimizing nanoscale fabrication techniques, which involve the precise manipulation and assembly of materials at the nanoscale. These techniques are essential for the production of nanoscale structures, devices, and systems with desired properties and functionalities. Computational models aid in the design, analysis, and optimization of fabrication processes, providing insights into the underlying physical and chemical phenomena. Here are some common computational modeling approaches for nanoscale fabrication techniques:

Finite Element Method (FEM):

The Finite Element Method is a numerical technique used to solve partial differential equations describing the behavior of materials and structures. FEM is widely employed to model various nanoscale fabrication processes, such as deposition, etching, and lithography. It allows for the simulation of material flow, heat transfer, and stress distribution, enabling the optimization of process parameters and the prediction of the resulting fabricated structures.

Molecular Dynamics (MD) Simulations:

Molecular Dynamics simulations model the behavior of individual atoms or molecules at the atomic scale, providing insights into nanoscale fabrication processes involving materials with discrete atomic arrangements. MD simulations are employed to study processes such as thin film growth, surface reactions, and nanoparticle self-assembly. By accounting for interatomic interactions and atomic-scale dynamics, MD simulations can predict the growth mechanisms, surface morphologies, and defects during fabrication processes.

Kinetic Monte Carlo (KMC) Simulations:

Kinetic Monte Carlo simulations track the stochastic motion and interaction of individual particles during fabrication processes. KMC simulations are particularly useful for understanding atomic-scale processes, such as surface diffusion, adsorption, desorption, and reaction kinetics. By considering the probabilities of various events and their time evolution, KMC simulations provide insights into the growth mechanisms, surface coverage, and crystallographic orientations during nanoscale fabrication.

Continuum Models:

Continuum models describe nanoscale fabrication processes as continuous fields, such as temperature, concentration, or stress distributions. These models use partial differential equations to capture the macroscopic behavior of the system during fabrication, including phenomena such as heat transfer, mass transport, and fluid flow. Continuum models, such as the Navier-Stokes equations or the heat equation, allow for the prediction of temperature profiles, material flow, and stress distribution during nanoscale fabrication.

Monte Carlo Simulations:

Monte Carlo simulations use random sampling techniques to model nanoscale fabrication processes. These simulations involve the probabilistic representation of the system, allowing for the exploration of a wide range of possible outcomes. Monte Carlo simulations are employed to study processes such as nanoparticle synthesis, surface patterning, and defect generation. By statistically sampling different events and outcomes, Monte Carlo simulations provide insights into the statistical properties and variability of fabricated structures.

Computational Fluid Dynamics (CFD):

Computational Fluid Dynamics techniques are used to model fluid flow and transport phenomena during nanoscale fabrication processes. CFD simulations enable the prediction of fluid behavior, mixing, and mass transport in fabrication techniques such as microfluidics and nanofluidics. By solving the Navier-Stokes equations, CFD simulations provide information on flow patterns, velocity profiles, and concentration distributions, aiding in the design and optimization of fabrication processes.

These computational modeling approaches are often combined with experimental data and theoretical models to enhance their accuracy and reliability. By simulating and analyzing nanoscale fabrication techniques, computational models provide valuable insights into the underlying physics and chemistry, optimize process parameters, and guide the development of novel fabrication strategies.

4. Nanoparticle Characterization and Properties

4.1. Modeling nanoparticle size, shape, and surface properties

Modeling nanoparticle size, shape, and surface properties is essential for understanding and predicting the characteristics of nanoparticles and tailoring their properties for specific applications [26]. Computational models are employed to simulate and analyze the factors that influence nanoparticle size, shape, and surface properties, considering various physical and chemical processes. Here are some common approaches to modeling nanoparticle size, shape, and surface properties:

Molecular Dynamics (MD) Simulations:

Molecular Dynamics simulations model the behavior of individual atoms or molecules in a nanoparticle system. By simulating the interactions between atoms and applying appropriate force fields, MD simulations can predict nanoparticle size, shape, and surface properties. These simulations allow for the exploration of various factors, such as temperature, pressure, and solvent effects, on nanoparticle morphology and stability.

Monte Carlo Simulations:

Monte Carlo simulations employ statistical sampling techniques to model the assembly and growth of nanoparticles. These simulations consider the probability of various events, such as particle attachment, detachment, and diffusion, to predict nanoparticle size, shape, and surface properties. Monte Carlo simulations are particularly useful for studying nanoparticle self-assembly, growth on surfaces, and the impact of different growth parameters on nanoparticle morphology.

Continuum Models:

Continuum models describe nanoparticle size, shape, and surface properties using macroscopic fields, such as concentration, temperature, and interfacial energy. These models use partial differential equations (PDEs) to simulate the growth and evolution of nanoparticles, taking into account mass transport, diffusion, and chemical reactions. Continuum models allow for the prediction of nanoparticle size distributions, shape transformations, and the influence of external conditions on nanoparticle morphology.

Crystal Growth Models:

Crystal growth models focus on the growth of crystalline nanoparticles. These models consider the dynamics of crystal growth, including surface kinetics, crystallographic orientations, and the impact of supersaturation or solution conditions. Crystal growth models, such as the Burton-Cabrera-Frank (BCF) model or phase-field models, simulate the growth and shape evolution of nanoparticles with crystalline structures, enabling the prediction of nanoparticle morphology and crystallographic features.

Shape-Control Models:

Shape-control models focus on predicting and controlling the shape of nanoparticles. These models consider factors such as surface energy, crystallographic anisotropy, and capping ligands or surfactants. By analyzing the balance between surface energies and crystallographic properties, shape-control models can provide insights into the growth conditions and mechanisms for obtaining specific nanoparticle shapes, such as rods, cubes, or polyhedra.

Empirical Models:

Empirical models are data-driven models that correlate experimental observations with nanoparticle size, shape, and surface properties. These models use statistical analysis and machine learning techniques to establish relationships between synthesis parameters, precursor concentrations, and resulting nanoparticle characteristics. Empirical models can provide predictive capabilities and guide experimental efforts to achieve desired nanoparticle properties.

It is important to note that the accuracy and reliability of these models depend on the underlying assumptions, available data, and the complexity of the nanoparticle system. Models are often validated against experimental data to assess their predictive capabilities. Combining computational modeling with experimental characterization techniques allows for a comprehensive understanding of nanoparticle size, shape, and surface properties and

facilitates the design and optimization of nanoparticles for various applications in materials science, catalysis, and nanomedicine [27].

4.2.Characterization techniques and mathematical analysis

Characterization techniques and mathematical analysis play a crucial role in understanding and quantifying the properties of materials and systems. These techniques allow researchers to obtain experimental data and measurements, which can then be subjected to mathematical analysis to extract meaningful information and insights. Here are some commonly used characterization techniques and mathematical analysis methods:

Characterization Techniques:

Scanning Electron Microscopy (SEM): SEM provides high-resolution images of the surface morphology of materials, enabling the measurement of particle size, shape, and surface features.

Transmission Electron Microscopy (TEM): TEM provides detailed information about the internal structure of materials at the atomic scale. It allows for the measurement of particle size, lattice spacing, and crystallographic features.

X-ray Diffraction (XRD): XRD is used to determine the crystal structure and composition of materials by analyzing the scattering of X-rays. It provides information about crystallographic phases, lattice parameters, and grain size.

Fourier Transform Infrared Spectroscopy (FTIR): FTIR measures the absorption and transmission of infrared light by materials, providing information about chemical composition, functional groups, and molecular vibrations.

Nuclear Magnetic Resonance (NMR): NMR measures the interaction of atomic nuclei with a magnetic field and provides information about molecular structure, chemical bonding, and dynamics.

Atomic Force Microscopy (AFM): AFM measures forces between a sharp probe and the sample surface, allowing for high-resolution imaging and measurement of surface roughness, topography, and mechanical properties.

Mathematical Analysis Methods:

Statistical Analysis: Statistical analysis techniques, such as mean, variance, and correlation analysis, provide insights into the distribution, trends, and relationships within datasets. These methods allow researchers to identify patterns, quantify uncertainties, and assess the significance of experimental results [28].

Regression Analysis: Regression analysis involves fitting mathematical models to experimental data to establish relationships between variables. It allows for the estimation of parameters, prediction of unknown values, and identification of trends or correlations.

Fourier Transform Analysis: Fourier transform is used to decompose complex signals or functions into their frequency components. It allows for the analysis of periodic patterns, spectral characteristics, and the extraction of relevant information from signals or spectra.

Numerical Optimization: Numerical optimization methods, such as gradient descent, genetic algorithms, or simulated annealing, are employed to find optimal solutions or parameter values that minimize or maximize an objective function. These methods are useful for parameter estimation, model fitting, and optimization problems.

Data Visualization: Data visualization techniques, including plots, graphs, and diagrams, provide a visual representation of experimental data. They aid in the interpretation and communication of complex data patterns, trends, and relationships.

Computational Modeling: Computational modeling involves using mathematical equations, simulations, or algorithms to represent and analyze complex systems. It enables the prediction of system behavior, optimization of parameters, and exploration of scenarios that are difficult or costly to study experimentally.

4.3. Predictive modeling of nanoparticle behavior

Predictive modeling of nanoparticle behavior involves developing mathematical and computational models that can accurately predict the properties and behavior of nanoparticles under different conditions. These models are based on fundamental principles, empirical data, and experimental observations, and they enable researchers to understand and predict various aspects of nanoparticle behavior. Here are some key considerations and approaches for predictive modeling of nanoparticle behavior:

Size and Shape Effects:

Nanoparticles exhibit unique size and shape-dependent properties due to quantum confinement, surface effects, and altered surface-to-volume ratios. Predictive models should consider these effects by incorporating appropriate size and shape descriptors, such as nanoparticle diameter, aspect ratio, or surface area-to-volume ratio. Theoretical models, empirical relationships, and machine learning algorithms can be employed to establish the relationships between nanoparticle size, shape, and various properties, such as optical, electronic, or catalytic behavior.

Surface Chemistry and Functionalization:

Nanoparticle surfaces play a crucial role in their behavior and interactions with the environment. Modeling the surface chemistry and functionalization of nanoparticles is essential for understanding their stability, reactivity, and surface-related phenomena. Models can incorporate surface energy, ligand interactions, and surface coverage to predict the behavior of functionalized nanoparticles in different solvents, environments, or biological systems. Quantum mechanical calculations, molecular dynamics simulations, and empirical parameterization can be used to model surface chemistry and functionalization effects [29].

Interparticle Interactions:

Nanoparticles often interact with each other, leading to collective behavior, assembly, or aggregation. Predictive models should consider interparticle interactions, including van der Waals forces, electrostatic interactions, steric effects, and magnetic interactions. These models can range from simplified analytical models, such as DLVO theory, to more complex simulations, such as Monte Carlo or molecular dynamics simulations, that capture the detailed interaction potentials and kinetics of nanoparticle interactions. The models enable the prediction of nanoparticle assembly, aggregation, and stability in different environments.

Environmental Factors:

Nanoparticle behavior is influenced by environmental factors such as temperature, pH, solvent properties, and exposure to external stimuli. Predictive models should account for these factors and their impact on nanoparticle properties and behavior. Thermodynamic models, reaction kinetics models, or machine learning algorithms can be employed to

capture the relationships between environmental factors and nanoparticle behavior, allowing for predictions under different conditions.

Multiscale Modeling:

Nanoparticles often exhibit behavior that spans multiple length and time scales. Multiscale modeling approaches, such as hierarchical modeling, coarse-graining, or coupling different modeling techniques, can be employed to capture these multiscale phenomena. These models integrate different levels of description, from atomistic simulations to continuum models, to predict nanoparticle behavior across different scales. The models enable the prediction of the influence of microstructural features, such as defects, grain boundaries, or surface roughness, on the properties and behavior of nanoparticles.

Validation and Iterative Refinement:

Predictive models of nanoparticle behavior should be validated against experimental data and benchmark cases to ensure their accuracy and reliability. Comparison with experimental results allows for model refinement and improvement. Models can be iteratively refined by incorporating new data, adjusting parameters, or incorporating additional physical phenomena to enhance their predictive capabilities.

5. Nanofluidics and Transport Phenomena

5.1. Mathematical modeling of fluid flow at the nanoscale

Mathematical modeling of fluid flow at the nanoscale involves describing and predicting the behavior of fluids in confined geometries or at the molecular level. Fluid flow at the nanoscale is characterized by unique phenomena, such as slip flow, surface effects, and molecular interactions, which require specialized mathematical models to capture the underlying physics. Here are some common approaches to mathematical modeling of fluid flow at the nanoscale [30]:

Navier-Stokes Equations:

The Navier-Stokes equations form the basis for modeling fluid flow at various length scales, including the nanoscale. However, at the nanoscale, the assumptions underlying the Navier-Stokes equations may no longer hold, and additional considerations are required. Extensions of the Navier-Stokes equations, such as the modified Navier-Stokes equations or the Burnett equations, can incorporate slip boundary conditions, non-continuum effects, and rarefaction phenomena observed at the nanoscale.

Molecular Dynamics (MD) Simulations:

Molecular Dynamics simulations model fluid flow at the atomic or molecular level, capturing the interactions and movements of individual particles. These simulations consider intermolecular forces, thermal effects, and particle motion to predict fluid behavior. MD simulations are particularly useful for studying fluid flow in nanochannels, nanoscale porous media, or systems where molecular interactions dominate. They provide insights into velocity profiles, diffusion, and fluid properties at the nanoscale.

Lattice Boltzmann Method (LBM):

The Lattice Boltzmann Method is a computational technique used to simulate fluid flow by discretizing the fluid into a lattice and tracking particle distribution functions. LBM is efficient for modeling complex geometries and can capture non-continuum effects, slip flow, and mesoscopic phenomena. LBM is often employed to study fluid flow in nanochannels, nanoporous materials, or microfluidic devices at the nanoscale.

Slip Flow Models:

At the nanoscale, fluid flow near solid surfaces can exhibit slip boundary conditions, where the fluid velocity at the surface differs from that predicted by classical hydrodynamics. Slip flow models, such as the Navier slip condition or the molecular kinetic theory, incorporate slip boundary conditions to describe the flow behavior near solid surfaces. These models account for surface interactions, intermolecular forces, and surface roughness effects.

Nanofluidics and Electrokinetics Models:

Nanofluidics models are specifically designed to describe fluid flow in nanoscale channels, pores, or devices. These models consider the unique characteristics of nanoscale confinement, electrokinetic effects, and surface charges. Models such as the Poisson-Boltzmann equation, Nernst-Planck equation, or the electroosmotic flow equations are employed to describe fluid behavior and ion transport in nanofluidic systems.

Non-equilibrium Statistical Mechanics:

Non-equilibrium statistical mechanics provides a theoretical framework for modeling fluid flow at the nanoscale, considering the deviations from equilibrium and the non-continuum effects. These models, such as the Boltzmann equation, provide a microscopic description of fluid flow, incorporating molecular interactions, collisions, and energy transfer. They are particularly suitable for studying rarefied gas flows or fluid flow in extremely confined geometries.

5.2. Nanofluidic devices and their design optimization

Nanofluidic devices are microscale or nanoscale structures that manipulate fluids at the molecular or nanoscale level. These devices have unique properties and functionalities that make them valuable for various applications, such as lab-on-a-chip systems, chemical analysis, DNA sequencing, drug delivery, and energy conversion. Design optimization of nanofluidic devices involves maximizing device performance, enhancing fluid manipulation capabilities, and tailoring device properties for specific applications. Here are some key considerations and approaches for nanofluidic device design optimization [30]:

Device Geometry and Channel Design:

The geometry and design of nanofluidic channels significantly impact fluid flow behavior, mass transport, and device performance. Design optimization involves considering factors such as channel dimensions, aspect ratios, surface roughness, and electrode configurations. Computational fluid dynamics (CFD) simulations, analytical models, and empirical correlations can be employed to analyze and optimize channel geometries to achieve desired fluid flow characteristics, minimize pressure drop, and enhance transport efficiency.

Surface Modification and Functionalization:

Surface properties play a crucial role in nanofluidic devices, influencing fluid-surface interactions, wettability, and surface charge. Surface modification techniques, such as chemical functionalization, nanoparticle deposition, or polymer coatings, can be utilized to tailor surface properties. Design optimization involves selecting appropriate surface modifications to control fluid behavior, enhance selectivity, reduce fouling, and improve device performance. Theoretical models and molecular simulations can guide the selection and optimization of surface modifications.

Electrokinetic and Electrophoretic Effects:

Electrokinetic phenomena, such as electroosmosis, electrophoresis, and dielectrophoresis, are commonly utilized in nanofluidic devices for fluid manipulation, particle separation,

and concentration enrichment. Design optimization involves optimizing electrode configurations, potential gradients, and buffer conditions to enhance electrokinetic effects and achieve efficient fluid control. Numerical simulations, analytical models, and experimental optimization techniques can be employed to optimize electrode designs and control parameters.

Material Selection:

The choice of materials for nanofluidic devices is crucial for device performance, compatibility with target fluids, and resistance to fouling. Materials should exhibit low autofluorescence, chemical stability, and biocompatibility when necessary. Optimization involves selecting suitable materials, such as glass, silicon, polymers, or metal oxides, based on their mechanical properties, surface characteristics, and manufacturing feasibility.

Integration and System-Level Optimization:

Nanofluidic devices are often integrated with other components or systems, such as microfluidic networks, sensing elements, or external control units. System-level optimization involves considering the interactions between the nanofluidic device and the larger system, optimizing fluid connections, sensor placement, and control strategies. Mathematical modeling, design of experiments (DOE), and multi-objective optimization techniques can be employed to optimize the overall system performance and achieve desired functionalities [31].

Fabrication and Manufacturing Optimization:

The fabrication and manufacturing processes for nanofluidic devices significantly impact device performance, reproducibility, and scalability. Optimization involves selecting appropriate fabrication techniques, such as lithography, nanoimprint, or self-assembly, and optimizing process parameters to achieve precise channel dimensions, surface quality, and device uniformity. Process modeling, design of experiments, and statistical analysis techniques can be employed to optimize fabrication processes and achieve high-quality nanofluidic devices.

5.3. Transport phenomena in nanochannels and nanoscale confinement

Transport phenomena in nanochannels and nanoscale confinement refer to the unique behaviors and characteristics exhibited by fluids when confined to nanoscale dimensions. These phenomena arise due to the dominance of surface effects, molecular interactions, and restricted molecular motion in the confined space. Understanding and modeling these transport phenomena are crucial for designing and optimizing nanofluidic devices, nanoscale separations, and nanofluidic systems. Here are some key transport phenomena observed in nanochannels and nanoscale confinement:

Slip Flow:

Slip flow is a phenomenon where the fluid velocity at the channel walls differs from that predicted by classical hydrodynamics. In nanochannels, fluid molecules experience interactions with the solid walls that can cause them to slip or slide along the wall surface, resulting in a slip velocity. Slip flow can significantly affect fluid flow rates, pressure drops, and mass transport in nanochannels. Slip length, which quantifies the extent of slip at the wall, plays a crucial role in modeling slip flow behavior.

Knudsen Flow and Rarefied Gas Effects:

When the characteristic dimensions of the channel are comparable to or smaller than the mean free path of gas molecules, the gas flow enters the Knudsen flow regime. In this regime, molecular collisions become important, and continuum assumptions of fluid flow break down. Knudsen flow leads to rarefied gas effects, including non-equilibrium velocity distributions, thermal creep, and diffusion phenomena that differ from those in the continuum regime.

Surface Wetting and Capillary Effects:

Surface wetting and capillary effects are particularly significant in nanochannels and nanoscale confinement. The interaction between the fluid and the channel surface can result in capillary forces, wetting behavior, and meniscus formation. These effects influence the flow behavior, spreading dynamics, and surface tension of the fluid in the confined space. They play a crucial role in processes such as droplet formation, liquid spreading, and wetting transitions in nanochannels.

Electroosmosis and Electrophoresis:

Electroosmosis and electrophoresis are electrokinetic phenomena that occur in nanochannels when an electric field is applied. Electroosmosis refers to the motion of the fluid induced by the electric field, while electrophoresis describes the movement of charged particles or solutes in the electric field. In nanochannels, these phenomena can be significantly enhanced due to the high surface-to-volume ratio, resulting in efficient fluid control, particle manipulation, and separation capabilities.

Confinement and Surface Effects on Diffusion:

Diffusion of molecules in nanochannels and nanoscale confinement is influenced by the confinement itself and the interactions with the channel walls. The restricted space can lead to hindered or enhanced diffusion rates compared to bulk conditions. Surface interactions and adsorption can affect the diffusion coefficients, solute transport, and separation selectivity. Understanding these effects is crucial for accurate modeling and design of nanofluidic systems.

Thermal and Energy Transport:

Heat and energy transport in nanochannels exhibit unique characteristics due to the strong confinement and surface interactions. Heat transfer mechanisms such as conduction, convection, and radiation are influenced by the channel geometry, surface properties, and molecular interactions. Nanoscale confinement can lead to enhanced heat transfer, reduced thermal conductivity, and modified temperature profiles, impacting heat dissipation, energy conversion, and thermal management in nanofluidic devices.

6. Nanoelectronics and Nanoscale Devices

6.1. Modeling charge transport in nanoscale electronic devices

Modeling charge transport in nanoscale electronic devices involves understanding and predicting the behavior of electrical current and charge carriers at the nanoscale. These devices, such as nanowires, nanotubes, or molecular junctions, exhibit unique quantum mechanical effects and size-dependent properties that require specialized models to capture their electronic transport characteristics. Here are some key considerations and approaches for modeling charge transport in nanoscale electronic devices [32]:

Quantum Transport Models:

At the nanoscale, quantum mechanical effects become prominent, and wave-like behavior of electrons needs to be considered. Quantum transport models, such as the non-equilibrium Green's function (NEGF) formalism or the tight-binding approach, describe the electron transport through nanoscale devices by incorporating the electronic band structure, quantum states, and scattering mechanisms. These models allow for the calculation of current-voltage characteristics, conductance, and transmission probabilities through the device.

Landauer-Büttiker Formalism:

The Landauer-Büttiker formalism provides a framework for modeling coherent electron transport in nanoscale devices. It treats the device as a scattering region connected to electron reservoirs, and the transport properties are determined by the transmission probabilities of electrons through the device. The Landauer formula relates the electrical current to the transmission probabilities and the applied voltage bias, enabling the calculation of current-voltage characteristics and conductance.

Density Functional Theory (DFT):

Density Functional Theory is a widely used computational method for modeling electronic structure and properties of materials at the nanoscale. DFT can be employed to calculate the electronic structure, energy levels, and transport properties of nanoscale electronic devices. Combined with transport models, DFT can provide insights into charge carrier distributions, conductance, and current flow through nanoscale systems.

Nonequilibrium Green's Function (NEGF) Method:

The Nonequilibrium Green's Function method is a powerful technique for modeling electron transport in nanoscale electronic devices. NEGF combines quantum mechanics and statistical mechanics to describe electron transport under nonequilibrium conditions. It allows for the calculation of current-voltage characteristics, transmission probabilities, and energy-dependent conductance through nanoscale devices. NEGF is particularly suitable for studying the effects of device geometry, scattering, and electron-electron interactions on charge transport.

Molecular Dynamics Simulations:

Molecular Dynamics simulations, coupled with electronic structure calculations, can be used to model charge transport in nanoscale devices with atomic-level detail. These simulations track the motion and interactions of individual atoms and electrons, allowing for the investigation of electron transport mechanisms, scattering events, and device behavior. Molecular Dynamics simulations provide insights into the dynamics of charge carriers, energy dissipation, and conductance in nanoscale electronic devices.

Modeling Electron-Phonon Interactions:

In nanoscale electronic devices, interactions between electrons and lattice vibrations (phonons) can influence charge transport. Modeling electron-phonon interactions is important for understanding energy dissipation, heat generation, and thermal conductance in nanoscale devices. Various theoretical approaches, such as self-consistent Born approximation (SCBA), molecular dynamics with electron-phonon coupling, or nonequilibrium Green's function methods with electron-phonon interactions, can be employed to study electron-phonon interactions and their effects on charge transport.

6.2. Quantum transport models and simulations

Quantum transport models and simulations are computational techniques used to study the behavior of charge carriers, such as electrons or holes, in nanoscale devices, where quantum mechanical effects dominate. These models and simulations provide insights into the electronic properties, transport phenomena, and device characteristics of nanoscale electronic systems. Here are some commonly used quantum transport models and simulation techniques:

Non-Equilibrium Green's Function (NEGF) Method:

The NEGF method is a powerful theoretical framework for modeling quantum transport in nanoscale devices. It combines quantum mechanics and statistical mechanics to describe the propagation of charge carriers through a device under nonequilibrium conditions. NEGF takes into account the electronic structure, scattering mechanisms, and energy-dependent transmission probabilities. It enables the calculation of current-voltage characteristics, conductance, and quantum states of the system. NEGF is particularly suitable for systems with weakly coupled electrodes and allows for the study of coherent transport and quantum interference effects.

Tight-Binding Model:

The tight-binding model is a simplified approach that approximates the electronic structure of a nanoscale system using a set of localized atomic orbitals. It allows for the calculation of electronic band structures, density of states, and wave functions of charge carriers. The tight-binding model can be employed to study quantum transport phenomena in various nanoscale devices, including nanowires, nanotubes, and molecular junctions. It is computationally efficient and offers insights into the spatial distribution of charge carriers and their transport properties.

Density Functional Theory (DFT) Combined with NEGF:

Density Functional Theory is a first-principles method that describes the electronic structure and properties of materials based on the principles of quantum mechanics. When combined with NEGF, DFT allows for the calculation of quantum transport properties of nanoscale systems. It provides a self-consistent approach to calculate the electronic structure, scattering potentials, and transmission probabilities. DFT-NEGF simulations can reveal the energy-dependent conductance, quantum states, and transport characteristics of nanoscale electronic devices.

Wigner Function Method:

The Wigner function method is a semiclassical approach that combines quantum mechanics with classical phase space methods. It provides a phase-space representation of charge carrier distribution and dynamics, allowing for the simulation of quantum transport phenomena. The Wigner function method is particularly useful for studying transport in systems with strong electron-electron interactions, such as quantum dots or mesoscopic systems.

Quantum Monte Carlo (QMC) Simulations:

Quantum Monte Carlo simulations are stochastic methods that numerically solve the many-body Schrödinger equation to study quantum systems. QMC simulations provide accurate descriptions of electronic structures, correlation effects, and quantum transport properties. They can be used to investigate charge transport phenomena in complex nanoscale devices, including systems with strong electron-electron interactions and disorder.

Time-Dependent Density Functional Theory (TD-DFT):

TD-DFT is an extension of DFT that allows for the calculation of time-dependent electronic properties and excitations. It can be employed to study the dynamics of charge carriers, optical properties, and transport phenomena in nanoscale devices under time-varying electric fields or external perturbations. TD-DFT simulations provide insights into the response of nanoscale systems to applied electric fields and the generation of excitations during transport.

6.3. Design and optimization of nanoelectronic circuits

Design and optimization of nanoelectronic circuits involve the development of integrated circuits (ICs) and electronic systems at the nanoscale, where individual components and features are on the order of nanometers. Nanoelectronic circuits offer advantages such as increased functionality, higher performance, and reduced power consumption. Here are some key considerations and approaches for designing and optimizing nanoelectronic circuits:

Technology Selection:

The choice of nanoelectronic technology is a critical step in circuit design. Various nanoscale technologies, such as nanowire transistors, carbon nanotubes, or graphene-based devices, offer unique properties and performance characteristics. The technology selection depends on the desired circuit specifications, manufacturability, scalability, and compatibility with existing fabrication processes.

Transistor Design and Scaling:

Transistors are the building blocks of electronic circuits. Designing and optimizing nanoscale transistors involve considerations such as device scaling, gate length, channel dimensions, doping profiles, and material properties. Device simulations, compact models, and process simulation tools are employed to optimize transistor designs for improved performance, reduced power consumption, and increased packing density.

Circuit Architecture and Topology:

Circuit architecture and topology define the interconnections and organization of circuit components. Optimizing circuit architecture involves selecting the appropriate topology, hierarchical design, and partitioning of functional blocks. Techniques such as clocking, pipelining, and parallelism are employed to optimize circuit performance, power consumption, and speed.

Power and Signal Integrity:

Power and signal integrity are critical factors in nanoelectronic circuit design. Power optimization techniques, such as power gating, voltage scaling, and dynamic voltage and frequency scaling (DVFS), are employed to reduce power consumption. Signal integrity considerations involve minimizing noise, crosstalk, and delay variations through techniques like shielding, decoupling capacitors, and impedance matching.

Design for Manufacturability (DFM):

Design for Manufacturability techniques ensure that the circuit can be reliably manufactured within the limits of fabrication processes. DFM considerations include design rules, lithography limits, process variations, and yield optimization. Design rules are tailored to the specific nanoelectronic technology, allowing for efficient and manufacturable circuit layouts.

Timing and Performance Optimization:

Timing and performance optimization techniques aim to improve the speed and efficiency of nanoelectronic circuits. Techniques such as static timing analysis, clock tree synthesis, and logic synthesis tools are employed to optimize critical paths, reduce delays, and achieve desired performance specifications. Trade-offs between speed, power consumption, and area are considered during optimization.

Noise and Variability Analysis:

Nanoelectronic circuits are susceptible to noise and variability due to process variations, thermal effects, and environmental conditions. Analysis and mitigation of noise sources, such as thermal noise, shot noise, and process-induced variations, are essential for ensuring circuit reliability and performance. Statistical analysis tools, such as Monte Carlo simulations and statistical timing analysis, are employed to evaluate and mitigate variability effects.

Testability and Reliability:

Designing nanoelectronic circuits with testability and reliability in mind is crucial. Built-in self-test (BIST) techniques, error correction codes, and redundancy schemes are employed to enhance testability and fault tolerance. Reliability considerations involve analyzing aging effects, electromigration, and thermal management to ensure long-term circuit operation.

7. Nanomedicine and Drug Delivery

7.1. Mathematical models for drug delivery systems

Mathematical models play a crucial role in understanding and optimizing drug delivery systems. These models provide insights into drug release kinetics, transport mechanisms, and the interaction between drugs and biological systems. Here are some common mathematical models used in drug delivery systems [33-35]:

Diffusion Models:

Diffusion models describe the transport of drugs through a medium, such as a polymer matrix or biological tissue, by considering Fick's laws of diffusion. These models assume that drug transport occurs solely through concentration gradients. Diffusion models are often employed to describe drug release from controlled-release systems, such as drug-loaded nanoparticles or implants. They allow for the prediction of drug release profiles, diffusion coefficients, and the impact of system parameters on drug release kinetics.

Pharmacokinetic Models:

Pharmacokinetic models focus on the distribution, absorption, metabolism, and excretion of drugs in the body. These models describe the time course of drug concentrations in different tissues and compartments. Pharmacokinetic models incorporate physiological parameters, such as blood flow rates, organ volumes, and drug clearance rates, to predict drug concentrations over time. They are useful for optimizing drug dosing regimens and predicting drug behavior in different patient populations.

Compartmental Models:

Compartmental models divide the body into compartments and describe the movement of drugs between these compartments. Each compartment represents a distinct physiological or anatomical region, such as blood, tissue, or organs. Compartmental models utilize differential equations to model drug transport and exchange between compartments. These

models are employed to analyze drug distribution, elimination, and multi-compartmental pharmacokinetics.

Target Site Models:

Target site models focus on the interaction between drugs and specific target sites within the body, such as tumor tissue or receptor sites. These models consider factors such as drug-receptor binding, drug internalization, and downstream signaling pathways. Target site models can be based on mass action kinetics or receptor-ligand binding models to predict drug-target interactions, drug efficacy, and dose-response relationships.

Population Pharmacokinetic Models:

Population pharmacokinetic models consider inter-individual variability in drug pharmacokinetics within a population. These models account for variations in physiological parameters, genetic factors, and disease states among individuals. Population pharmacokinetic models utilize population-based statistical analysis techniques, such as mixed-effects modeling, to describe the population mean and individual variability in drug concentrations over time. They are valuable for individualized dosing regimens and dose adjustment in patient populations.

Computational Fluid Dynamics (CFD) Models:

CFD models simulate the flow of fluids, such as blood or drug solutions, in complex geometries, such as blood vessels or microfluidic devices. CFD models incorporate Navier-Stokes equations, mass transport equations, and boundary conditions to predict fluid flow patterns, drug dispersion, and local drug concentrations. CFD models provide insights into drug transport in vasculature, local drug delivery, and the impact of fluid dynamics on drug distribution [34].

7.2. Pharmacokinetic and pharmacodynamic modelling

Pharmacokinetic and pharmacodynamic (PK/PD) modeling is a quantitative approach used to characterize the relationship between drug concentrations in the body (pharmacokinetics) and the resulting drug effects (pharmacodynamics). PK/PD modeling plays a crucial role in drug development, dosage optimization, and understanding drug-response relationships. Here's an overview of pharmacokinetic and pharmacodynamic modeling:

Pharmacokinetic Modeling:

Pharmacokinetic modeling focuses on the quantitative description of drug absorption, distribution, metabolism, and elimination (ADME) within the body. It involves the development of mathematical models that describe the time course of drug concentrations in various tissues, organs, and compartments. Some commonly used pharmacokinetic models include:

Compartmental Models: Compartmental models divide the body into distinct compartments and describe drug movement between these compartments using ordinary differential equations. Each compartment represents a physiological or anatomical region, such as the blood, liver, or kidneys. Compartmental models can be simple (one or two compartments) or more complex (multi-compartmental) to account for different drug distribution and elimination processes.

Physiologically Based Pharmacokinetic (PBPK) Models: PBPK models incorporate physiological and anatomical parameters, such as blood flow rates, tissue volumes, and organ-specific drug transport mechanisms, to simulate drug distribution and elimination.

These models consider drug-specific physicochemical properties, such as lipophilicity and protein binding, and provide a more mechanistic representation of drug pharmacokinetics.

Nonlinear Mixed-Effects Models: Nonlinear mixed-effects models are used to describe population-based pharmacokinetics, considering both inter-individual and intra-individual variability. These models account for variations in drug disposition among individuals, incorporating random effects and covariates such as age, body weight, or genetic factors.

Pharmacodynamic Modeling:

Pharmacodynamic modeling focuses on quantifying the relationship between drug concentrations and the resulting pharmacological effects. It aims to describe the concentration-effect relationship and the time course of drug response. Pharmacodynamic models can be classified into several types:

E_{max} Models: E_{max} models describe the relationship between drug concentration and the maximum effect achievable by the drug. These models assume a sigmoidal concentration-effect relationship, with the maximum effect (E_{max}) reached at a certain drug concentration (EC₅₀). E_{max} models are commonly used for drugs with reversible effects.

Receptor Binding Models: Receptor binding models describe the interaction between drugs and their target receptors. These models incorporate drug-receptor binding kinetics, receptor occupancy, and downstream signaling pathways to quantify drug effects. They can account for factors such as drug affinity, drug-receptor dissociation, and receptor desensitization.

Transduction Models: Transduction models describe the cellular or physiological processes that mediate the drug response. These models capture the drug's effect on biochemical pathways, enzyme kinetics, or signal transduction cascades. Transduction models can be based on ordinary differential equations, enzyme kinetics, or systems biology approaches.

Systems Pharmacology Models: Systems pharmacology models aim to integrate pharmacokinetics, pharmacodynamics, and disease biology to understand complex drug-response relationships. These models incorporate multiple physiological and biochemical pathways, disease-specific factors, and drug-target interactions to predict drug effects and optimize therapeutic interventions.

Pharmacokinetic and pharmacodynamic modeling are often performed together (PK/PD modeling) to provide a comprehensive understanding of the drug's behavior and effects. These models help in drug dosage optimization, predicting drug-response variability, understanding drug-drug interactions, and informing clinical decision-making.

7.3. Targeted drug delivery strategies at the nanoscale

Targeted drug delivery at the nanoscale involves the design and development of nanoscale delivery systems that can deliver drugs specifically to target sites in the body while minimizing off-target effects. These systems offer numerous advantages, such as improved drug solubility, prolonged drug circulation, enhanced drug stability, and controlled release kinetics. Here are some commonly used targeted drug delivery strategies at the nanoscale:

Passive Targeting:

Passive targeting relies on the enhanced permeability and retention (EPR) effect, which is characterized by the leaky vasculature and poor lymphatic drainage in tumor tissues. Nanoparticles, such as liposomes, micelles, or polymeric nanoparticles, can exploit the EPR effect to accumulate in tumor tissues by extravasation through leaky blood vessels.

These nanoparticles can deliver drugs selectively to tumor sites, taking advantage of the tumor microenvironment.

Active Targeting:

Active targeting involves the use of ligands, such as antibodies, peptides, or aptamers, that specifically recognize and bind to receptors overexpressed on target cells or tissues. These ligands are conjugated to the surface of nanocarriers to enable specific recognition and internalization by target cells. Active targeting can enhance the accumulation of nanoparticles at the desired site and improve drug delivery to target cells, leading to enhanced therapeutic efficacy.

Stimuli-Responsive Delivery Systems:

Stimuli-responsive delivery systems are designed to release drugs in response to specific environmental cues or stimuli at the target site. These stimuli can include changes in pH, temperature, enzymes, redox potential, or light. Nanoparticles are engineered with responsive components, such as pH-sensitive polymers, temperature-responsive lipids, or enzyme-cleavable linkers, to trigger drug release upon encountering the specific stimuli at the target site. This strategy allows for controlled drug release at the desired location, improving therapeutic outcomes.

Magnetic Targeting:

Magnetic targeting utilizes external magnetic fields to guide magnetic nanoparticles to specific target sites. Magnetic nanoparticles, such as iron oxide nanoparticles, are functionalized with drugs and guided to the target site using an external magnet. This approach is particularly useful in applications such as cancer therapy, where magnetic nanoparticles can be directed to the tumor site, leading to localized drug delivery and reduced systemic side effects.

Cell-Mediated Targeting:

Cell-mediated targeting involves utilizing specific cell types, such as immune cells or stem cells, as carriers to deliver drugs to target sites. These cells can be loaded with nanoparticles or drugs and administered systemically. The cells naturally migrate to specific tissues or sites of inflammation, allowing for targeted delivery. This strategy takes advantage of the natural homing capabilities of specific cell types, enabling precise drug delivery to desired locations.

Nanoscale Implants and Devices:

Nanoscale implants and devices provide a platform for targeted drug delivery directly at the site of interest. These implants can be designed to release drugs in a controlled and sustained manner, ensuring local drug delivery. Examples include drug-eluting stents, microneedle patches, or implantable nanoparticles. These devices are positioned at the target site, providing localized drug release and minimizing systemic side effects.

8. Challenges and Future Perspectives

8.1. Limitations and challenges in nanoscale mathematical modelling

While nanoscale mathematical modeling is a valuable tool for understanding and optimizing nanoscale systems, it also faces certain limitations and challenges. Here are some key limitations and challenges associated with nanoscale mathematical modeling:

Complexity of Systems:

Nanoscale systems often exhibit complex behaviors and interactions due to the intricate nature of nanoscale phenomena. Modeling such systems requires capturing various factors, including quantum effects, surface effects, molecular interactions, and multi-scale phenomena. The complexity of these systems poses challenges in developing accurate and computationally efficient mathematical models that can encompass all relevant factors.

Lack of Experimental Data:

Validating nanoscale mathematical models can be challenging due to limited experimental data at the nanoscale. Obtaining accurate and comprehensive experimental data at the nanoscale is often difficult and expensive. As a result, model calibration and validation may rely on limited experimental data, reducing the confidence in model predictions. The lack of experimental data also limits the ability to explore and account for system-specific or material-specific effects.

Uncertainty and Parameter Estimation:

Estimating model parameters accurately is crucial for reliable predictions. However, nanoscale systems often involve uncertain or poorly defined parameters, such as surface properties, intermolecular forces, or system-specific characteristics. Obtaining accurate parameter values and quantifying uncertainties can be challenging, which may affect the accuracy and robustness of model predictions. Advanced techniques, such as Bayesian inference or sensitivity analysis, can help address parameter uncertainty to some extent.

Computational Complexity:

Nanoscale systems often require complex mathematical models that involve high-dimensional equations and intricate numerical algorithms. The computational resources needed to solve these models can be substantial. Simulating nanoscale systems with high spatial and temporal resolutions, or incorporating quantum effects, can be computationally demanding. Balancing accuracy and computational efficiency is a persistent challenge in nanoscale mathematical modeling.

Scale Transitions and Multiscale Modeling:

Nanoscale systems frequently exhibit multiscale behaviors, where phenomena at different length scales interact and influence each other. Modeling these multiscale systems requires integrating models across different length and time scales, which can be challenging. Bridging models from atomistic simulations to continuum models or connecting models with different levels of complexity adds complexity and uncertainty to the modeling process.

Limited Model Transferability:

Models developed for specific nanoscale systems or materials may have limited transferability to other systems or materials. Nanoscale phenomena are highly dependent on system-specific or material-specific characteristics, making it difficult to generalize models across different systems. The lack of universal models hampers the ability to predict nanoscale behaviors accurately in diverse contexts.

8.2. Future directions for advancing mathematical modeling in nanotechnology

Advancing mathematical modeling in nanotechnology is crucial for deeper insights into nanoscale phenomena, guiding experimental design, and optimizing nanoscale systems. The government organizations have reported the worldwide investment on nanotechnology research around \$8.6 billion in 2004 [36], and it has increased to \$158.98 billion in 2021 to \$172.89 billion in 2022 (<https://www.globenewswire.com/news->

[release/2021/12/30/2359099/0/en/Nanotechnology-Services-Global-Market-Report-2022.html](https://www.researchandmarkets.com/2021/12/30/2359099/0/en/Nanotechnology-Services-Global-Market-Report-2022.html)) [37]. Here are some potential future directions for advancing mathematical modeling in nanotechnology:

Multi-scale Modeling and Integration:

Efforts can be directed towards developing and refining multi-scale modeling approaches that bridge different length and time scales, such as atomistic to continuum models. Integrating models across scales will enable a more comprehensive understanding of nanoscale systems and their behavior. Techniques like data-driven modeling, coarse-graining methods, and hybrid modeling approaches can be explored to improve the accuracy and efficiency of multi-scale simulations.

Quantum and Statistical Mechanics Modeling:

Advancements in modeling techniques that incorporate quantum mechanical effects and statistical mechanics will be instrumental in accurately capturing the behaviors of nanoscale systems. Improving quantum transport models, developing efficient methods for simulating quantum phenomena, and accounting for quantum coherence and entanglement effects will provide more accurate descriptions of nanoscale electronic and transport properties.

Data-Driven and Machine Learning Approaches:

The integration of data-driven approaches and machine learning techniques can complement traditional modeling approaches in nanotechnology. Machine learning algorithms can analyze large datasets, extract patterns, and facilitate predictive modeling. Combining experimental data with mathematical models through data assimilation techniques will enhance model accuracy and reduce uncertainties. Machine learning algorithms can also help optimize and accelerate computational simulations, improving efficiency and enabling high-throughput screening of nanomaterials and devices.

Uncertainty Quantification and Sensitivity Analysis:

Efforts can be directed towards enhancing uncertainty quantification techniques and sensitivity analysis in nanoscale modeling. Reliable estimation of uncertainties and sensitivities will provide insights into the reliability of model predictions and guide experimental design. Advanced statistical techniques, surrogate modeling, and global sensitivity analysis methods can be employed to better understand and quantify uncertainties and sensitivities in nanoscale models.

Inclusion of Dynamic and Non-equilibrium Effects:

Expanding modeling capabilities to account for dynamic and non-equilibrium effects in nanoscale systems will be essential. Many nanoscale processes, such as chemical reactions, phase transitions, and energy transport, occur far from equilibrium. Developing models that capture non-equilibrium dynamics, time-dependent phenomena, and transient processes will enable a more accurate representation of nanoscale behaviors.

Integration of Modeling and Experimentation:

Further integration of modeling and experimentation will foster a feedback loop for knowledge generation and model validation. Collaborations between modelers and experimentalists can facilitate the design of experiments specifically tailored to validate and refine mathematical models. This iterative process of modeling, experimentation, and validation will enhance the reliability and applicability of nanoscale mathematical models.

Open and Collaborative Modeling Platforms:

Developing open-access platforms and repositories for sharing nanoscale models, simulation codes, and experimental data will foster collaboration, reproducibility, and

knowledge exchange within the nanotechnology community. Open-source software tools, collaborative platforms, and standardized model formats can enable researchers to build upon existing models and accelerate progress in nanoscale modeling.

Advancing mathematical modeling in nanotechnology requires a collaborative and interdisciplinary effort that combines expertise from mathematics, physics, chemistry, materials science, and engineering. These future directions will contribute to a more comprehensive understanding of nanoscale phenomena, facilitate the design of novel nanomaterials and devices, and drive the development of transformative technologies in nanotechnology.

9. Conclusion

Mathematical modeling plays a vital role in advancing our understanding of nanotechnology and its applications. It enables the exploration of complex nanoscale phenomena, the optimization of nanoscale systems, and the prediction of their behavior. Through mathematical models, researchers can gain insights into the fundamental principles governing nanoscale processes, design and optimize drug delivery systems, develop nanoelectronic circuits, and investigate fluid flow at the nanoscale, among many other applications.

While mathematical modeling in nanotechnology offers numerous benefits, it also faces challenges and limitations. Complex systems, lack of experimental data, uncertain parameters, computational complexity, and scale transitions pose hurdles that need to be overcome. However, ongoing advancements in multi-scale modeling, quantum mechanics modeling, data-driven approaches, and uncertainty quantification techniques provide promising avenues for future progress.

To further advance mathematical modeling in nanotechnology, interdisciplinary collaborations, integration of experimental data, and open-access platforms for sharing models and data are essential. By addressing the challenges and leveraging emerging techniques, mathematical modeling will continue to drive innovation in nanotechnology, leading to breakthroughs in areas such as targeted drug delivery, nanoelectronics, energy conversion, and environmental remediation. With the continuous refinement and development of mathematical models, we can unlock the full potential of nanotechnology and its impact on various fields of science and technology.

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