IJARSCT
International Journal of Advanced Research in Science, Communication and Technology
International Open-Access, Double-Blind, Peer-Reviewed, Refereed, Multidisciplinary Online Journal
ISSN: 2581-9429
Volume 6, Issue 4, February 2026
Impact Factor: 8.2

Review on Recent Advances in Computational Chemistry

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Abstract: *This review paper explores recent advances in computational chemistry, emphasizing breakthroughs from 2022 to 2025. Key developments include enhanced quantum chemistry methods, innovative molecular dynamics simulations, and the integration of machine learning techniques. These advances have significantly improved the accuracy and efficiency of chemical modeling, enabling deeper insights into molecular behavior and reaction mechanisms. Additionally, multiscale modeling approaches have expanded the applicability of computational tools across diverse chemical systems, from small molecules to complex biomaterials. The convergence of artificial intelligence with traditional computational methods is driving transformative changes, facilitating rapid predictions and novel molecular designs. This review highlights the impact of these technological advancements on drug discovery, materials science, and sustainable chemistry, underscoring the growing importance of computational approaches in modern chemical research*

Keywords: Computational Chemistry, Quantum Chemistry, Molecular Dynamics, Machine Learning, Multiscale Modeling, Electronic Structure, Artificial Intelligence

I. INTRODUCTION

Computational chemistry has emerged as a cornerstone of modern chemical research, providing powerful theoretical and computational tools to investigate molecular structures, properties, and reaction mechanisms with unprecedented detail. Over the past decade, the field has witnessed remarkable growth fuelled by advances in computational algorithms, hardware capabilities, and the integration of artificial intelligence (AI) and machine learning (ML) techniques. These developments have significantly enhanced the accuracy, efficiency, and scope of computational models, enabling researchers to address increasingly complex chemical problems that were previously intractable.The evolution of computational chemistry is closely tied to improvements in quantum chemistry methods, which form the theoretical foundation for understanding electronic structures and molecular interactions. Enhanced density functional theory (DFT) functionals and post-Hartree-Fock methods have improved the precision of electronic structure calculations, while emerging quantum computing technologies promise to revolutionize the field by tackling problems beyond the reach of classical computers.Simultaneously, molecular dynamics (MD) simulations have advanced to capture the dynamic behavior of molecules over extended timescales and larger spatial domains. Innovations such as ab initio MD, coarse-grained models, and GPU-accelerated simulations have expanded the applicability of MD to biomolecular systems, materials science, and chemical processes in complex environments.The integration of AI and ML into computational chemistry has opened new avenues for accelerating discovery and design. Machine learning potentials, generative models, and hybrid approaches combining physics-based simulations with data-driven techniques are transforming how molecular properties are predicted and optimized. These tools facilitate rapid screening of chemical space, prediction of reaction outcomes, and autonomous optimization of synthetic pathways.Moreover, multiscale modeling approaches that bridge atomistic simulations with continuum and mesoscale models are enabling comprehensive studies of chemical systems across different length and time scales. This holistic perspective is crucial for understanding phenomena in materials science, environmental chemistry, and catalysis.This introduction provides a detailed overview of the recent advances in computational chemistry, emphasizing the technological breakthroughs and

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their implications for future research. By highlighting the synergy between traditional computational methods and emerging AI-driven techniques, it underscores the transformative potential of computational chemistry in addressing grand challenges in science and technology.The subsequent sections of this review delve into specific advancements in quantum chemistry, molecular dynamics, machine learning applications, and multiscale modeling, illustrating how these innovations are shaping the future of chemical research and interdisciplinary collaboration.

II. RECENT ADVANCES

A. Quantum Chemistry Methods

Development of new density functional theory (DFT) functionals improving accuracy and applicability, including meta-GGA and range-separated hybrids that better capture electron correlation effects. These functionals have enhanced the predictive power of DFT, enabling more reliable simulations of complex molecular systems, including transition metal complexes and excited states.Enhanced post-Hartree-Fock methods such as coupled-cluster with perturbative triples (CCSD(T)) and multireference approaches for precise electronic structure calculations in strongly correlated systems. Recent algorithmic improvements and parallelization techniques have made these computationally intensive methods more accessible for larger molecules.Exploration of quantum computing algorithms like variational quantum eigen solvers (VQE) and quantum phase estimation (QPE) to solve complex electronic structure problems beyond classical capabilities. Although still in early stages, these quantum algorithms show promise for tackling problems such as electronic correlation in large molecules and reaction pathways.Implementation of machine learning techniques to optimize quantum chemical calculations, including ML-based exchange-correlation functionals and surrogate models for rapid property prediction. These approaches reduce computational cost while maintaining accuracy, facilitating high-throughput screening of chemical compounds.Advances in excited-state methods enabling better simulation of photochemical and photophysical processes, such as time-dependent DFT (TD-DFT) with improved functionals and multiconfigurational perturbation theories. These methods allow detailed studies of light-induced reactions and energy transfer mechanisms.Introduction of fragment-based quantum chemical methods that allow accurate calculations on large molecular systems by dividing them into manageable fragments, significantly reducing computational cost. Techniques like the fragment molecular orbital (FMO) method and divide-and-conquer approaches have been refined for biomolecular and materials applications.Development of real-time time-dependent DFT (RT-TDDFT) methods for simulating electron dynamics and ultrafast processes. These methods provide insights into electron transport, charge transfer, and non-equilibrium phenomena relevant to photovoltaics and photocatalysis.

B. Molecular Dynamics Simulations

Advances in ab initio molecular dynamics (AIMD) combining quantum mechanical calculations with classical MD to simulate chemical reactions and material properties with high accuracy. Recent developments include improved algorithms for better scalability and longer simulation times.Development of enhanced sampling techniques such as meta dynamics, umbrella sampling, and replica exchange molecular dynamics (REMD) to overcome energy barriers and explore rare events in complex systems.Utilization of GPU acceleration and high-performance computing to enable large-scale simulations of biomolecules, polymers, and materials, significantly reducing computational time.Integration of machine learning potentials, such as neural network potentials and Gaussian approximation potentials, to achieve near quantum accuracy at a fraction of the computational cost, facilitating simulations of larger systems and longer timescales.Application of coarse-grained models to study large biomolecular assemblies and materials, balancing computational efficiency with sufficient detail to capture essential physical properties.Development of hybrid quantum mechanics/molecular mechanics (QM/MM) methods for simulating enzymatic reactions and catalytic processes, allowing accurate treatment of active sites within complex environments.Advances in nonequilibrium molecular dynamics simulations to study transport phenomena, reaction kinetics, and response to external fields, providing insights into dynamic processes in chemical and biological systems.

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C. Machine Learning Applications in Computational Chemistry

Implementation of machine learning models for predicting molecular properties, reaction outcomes, and synthetic pathways, accelerating the discovery process.Development of generative models and reinforcement learning techniques for de novo molecular design, enabling the creation of novel compounds with desired properties.Use of ML-based force fields and potentials to improve the accuracy and efficiency of molecular simulations.Integration of data-driven approaches with traditional physics-based models to enhance predictive capabilities and interpretability.Application of natural language processing (NLP) techniques to extract chemical knowledge from literature and databases, facilitating automated hypothesis generation.Development of active learning frameworks to iteratively improve ML models with minimal computational cost.Use of explainable AI methods to understand model decisions and guide experimental validation.

D. Multiscale Modeling

Advances in coupling atomistic simulations with mesoscale and continuum models to study complex chemical systems across multiple length and time scales.Development of adaptive resolution schemes allowing seamless transition between different levels of detail within a single simulation.Application of multiscale approaches to materials design, catalysis, and biological systems, providing comprehensive insights into structure-function relationships.Integration of machine learning techniques to bridge scales and improve model accuracy.Use of coarse-grained models combined with all-atom simulations to study large biomolecular complexes and assemblies.Development of hierarchical modeling frameworks for environmental chemistry and reaction networks.

E. Computational Tools and Software

Overview of widely used computational chemistry software packages such as Gaussian, ORCA, VASP, GROMACS, LAMMPS, and CP2K, highlighting recent updates and capabilities.

Introduction to emerging AI-driven platforms and tools that facilitate automated workflows, high-throughput screening, and data management.

Discussion of cloud computing resources and collaborative platforms enhancing accessibility and scalability of computational chemistry research.

Emphasis on open-source initiatives promoting reproducibility and community-driven development.

III. CONCLUSION

Computational chemistry has undergone transformative advancements in recent years, driven by innovations in quantum chemistry methods, molecular dynamics simulations, machine learning applications, and multiscale modeling. These developments have expanded the scope and accuracy of computational studies, enabling researchers to tackle increasingly complex chemical problems with greater efficiency. The integration of artificial intelligence and high-performance computing has accelerated discovery processes, facilitating rapid predictions and novel molecular designs. As computational tools become more accessible and versatile, their impact on drug discovery, materials science, and sustainable chemistry continues to grow. Future directions point towards deeper integration of quantum computing, enhanced machine learning models, and more sophisticated multiscale frameworks, promising to further revolutionize the field. This review underscores the critical role of computational chemistry in advancing scientific knowledge and addressing global challenges.

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DOI: 10.48175/IJARSCT-31712