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Applications of High-Performance Computing (HPC) in Materials Simulation

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ABSTRACT: High-Performance Computing (HPC) has become a fundamental pillar of modern computational materials science, enabling the simulation and analysis of increasingly complex material systems with unprecedented accuracy and efficiency. The rapid advancement of HPC architectures, including petascale and exascale computing platforms, has significantly expanded the capabilities of materials modeling and simulation. This review provides a comprehensive overview of the role of HPC in materials research, covering its applications in first-principles calculations based on Density Functional Theory (DFT), molecular dynamics (MD) simulations, high-throughput materials discovery, and the investigation of nanomaterials and two-dimensional materials. The integration of HPC with advanced computational techniques has facilitated the exploration of electronic, magnetic, optical, mechanical, and thermodynamic properties of materials across multiple length and time scales. In addition, the review discusses the growing synergy between HPC and Artificial Intelligence (AI), highlighting the emergence of Materials Informatics as a powerful paradigm for data-driven materials design and accelerated materials discovery. Major materials simulation software packages optimized for HPC environments, including VASP, Quantum ESPRESSO, CASTEP, ABINIT, SIESTA, LAMMPS, GROMACS, CP2K, and nanoDCAL, are also examined. Furthermore, current challenges related to computational scalability, energy consumption, and infrastructure costs are analyzed, together with future perspectives involving exascale computing, next-generation GPU architectures, machine learning, and quantum computing. Overall, HPC continues to play a pivotal role in advancing materials research and is expected to remain an indispensable tool for the discovery, design, and optimization of advanced materials for future technological applications.

KEYWORDS: High-Performance Computing; Density Functional Theory; Molecular Dynamics; Materials Discovery; Computational Materials Science

1. INTRODUCTION

Over the past few decades, the rapid advancement of science and technology has driven an increasing demand for the development of novel materials capable of meeting the stringent requirements of emerging applications in electronics, renewable energy, sensing technologies, quantum computing, data storage, and biomedicine. The discovery and design of advanced materials with superior electronic, magnetic, optical, and mechanical properties have become major research priorities in modern materials science. Alongside conventional experimental approaches, computational modeling has emerged as an indispensable tool for investigating material structures and properties at the atomic scale, enabling the prediction and optimization of material performance prior to experimental synthesis. The integration of quantum-mechanical theories, numerical simulation techniques, and advanced computational resources has significantly reduced research time and experimental costs while accelerating the development of nextgeneration materials [1–2].

In computational materials science, methodologies such as Density Functional Theory (DFT), Molecular Dynamics (MD), Monte Carlo simulations, and multiscale modeling often involve solving problems with an enormous number of degrees of freedom. This challenge becomes particularly significant for nanomaterials, two-dimensional materials, transition-metal-containing systems, and large-scale structures consisting of thousands to millions of atoms, where computational complexity increases dramatically with system size and the desired level of accuracy. Consequently, conventional computing platforms are often unable to provide the

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computational power and memory capacity required for modern simulations. For this reason, High-Performance Computing (HPC) has become an indispensable foundation for next-generation materials research. HPC systems utilize thousands to millions of processing cores operating in parallel to perform scientific computations at extremely high speeds. Modern HPC infrastructures have already reached petascale performance (10^15 floating-point operations per second) and are rapidly advancing toward the exascale regime (10^18 floating-point operations per second), enabling the solution of computational problems that were previously considered intractable. The emergence of exascale supercomputers has opened unprecedented opportunities for simulating highly complex material systems, ranging from quantum-level electronic processes to multiscale phenomena involving interactions among electrons, phonons, electromagnetic fields, and surrounding environments [3–4].

At present, HPC plays a central role in large-scale materials discovery initiatives worldwide, including the Materials Project, the Open Quantum Materials Database (OQMD), and the AFLOW Consortium, where millions of first-principles calculations are performed to establish comprehensive materials databases for scientific research and technological development. Furthermore, the integration of HPC with Artificial Intelligence (AI) and data science is creating a new paradigm for materials design, enabling the rapid screening of millions of potential material structures within a fraction of the time required by traditional approaches. Such developments are transforming the way new materials are discovered, optimized, and deployed for practical applications.

Owing to its unparalleled computational power, large-scale parallel processing capability, and support for sophisticated simulation algorithms, HPC has become a cornerstone of modern computational materials science. As scientific challenges continue to expand in terms of system size, computational accuracy, and multiscale complexity, the importance of HPC is expected to grow further, driving future breakthroughs in the design and development of advanced materials for next-generation technologies [5].

2. HIGH-PERFORMANCE COMPUTING (HPC): CONCEPTS AND FUNDAMENTALS

High-Performance Computing (HPC) refers to a class of computing systems specifically designed to solve highly complex scientific and engineering problems by exploiting the parallel processing capabilities of multiple processors operating simultaneously. Unlike conventional personal computers, which are typically limited to a relatively small number of processing cores, HPC systems can incorporate thousands to millions of computational cores interconnected through highspeed communication networks. This architecture enables large computational tasks to be decomposed into smaller subtasks that can be executed concurrently across multiple computing nodes, thereby substantially reducing execution time and improving overall computational efficiency [6].

A modern HPC system typically consists of specialized hardware and software components, including high-performance central processing units (CPUs), graphics processing units (GPUs), large-capacity memory systems, high-speed storage devices, and dedicated interconnect technologies such as InfiniBand and Slingshot. In recent years, the integration of GPUs into HPC architectures has become a dominant trend due to their ability to execute thousands of parallel computational threads simultaneously. This capability is particularly advantageous for scientific simulations, artificial intelligence applications, and machine-learning workloads. The synergistic combination of CPUs and GPUs has significantly enhanced the computational performance of modern supercomputers while improving energy efficiency on a per-operation basis [7].

The performance of HPC systems is commonly measured in Floating Point Operations Per Second (FLOPS). Throughout the history of supercomputing, performance has increased exponentially, progressing from gigaflops (10^9 FLOPS) to teraflops (10^{12} FLOPS), petaflops (10^{15} FLOPS), and ultimately exaflops (10^{18} FLOPS). A major milestone in this evolution was achieved in 2022 with the deployment of the world's first exascale supercomputer, capable of performing more than one quintillion floating-point operations per second, thereby inaugurating a new era of large-scale scientific simulations [8].

In materials science research, HPC serves as the computational foundation for advanced simulation methodologies such as Density Functional Theory (DFT), Molecular Dynamics (MD), Monte Carlo simulations, and multiscale modeling. These approaches often require solving systems involving thousands or millions of variables, demanding substantial memory resources and prolonged computation times if performed on conventional computers. Through large-scale parallel processing, HPC enables highly accurate simulations of complex material systems, ranging from quantum-level electronic structures to mesoscale and macroscale physical phenomena. Such capabilities have significantly contributed to the discovery of novel materials, optimization of material properties, and advancement of computational materials science as a whole [3].

The emergence of exascale computing has not only increased computational capability but has also facilitated the integration of materials simulations with artificial intelligence, machine learning, and data-driven methodologies. These technologies are fostering a new research paradigm in which vast materials databases generated through millions of HPC calculations can be leveraged to predict and design novel materials at unprecedented speed and efficiency. Consequently, HPC is no longer merely a computational tool but has evolved into a strategic scientific infrastructure that underpins many of the world's most advanced materials research initiatives.

3. THE ROLE OF HIGH-PERFORMANCE COMPUTING (HPC) IN MATERIALS SIMULATION

3.1. First-Principles Calculations

One of the most important and widely adopted applications of High-Performance Computing (HPC) in materials science is the implementation of first-principles calculations, particularly those based on Density Functional Theory (DFT). Since the formulation of the foundational theorems by Hohenberg and Kohn, DFT has become the standard theoretical framework for investigating the electronic structure and physical properties of materials at the atomic scale. However, solving the Kohn–Sham equations for many-electron systems requires enormous computational resources, especially for materials with large simulation cells or systems containing strongly correlated electrons. Consequently, the development of HPC has played a crucial role in extending the applicability of DFT to increasingly complex materials science problems [9–10].

Widely used materials simulation packages such as VASP, Quantum ESPRESSO, CASTEP, ABINIT, SIESTA, and CP2K have all been developed with parallel computing architectures to efficiently exploit HPC resources. Through the distribution of calculations across reciprocal-space grids, Brillouin-zone k-points, energy bands, and computational nodes, HPC significantly reduces computational time while enabling the study of material systems containing hundreds to thousands of atoms. As a result, researchers can investigate electronic structures, band-gap energies, density of states (DOS), electronic band structures, magnetic properties, optical properties, formation energies, and thermodynamic stability with high accuracy [11–12].

The importance of HPC becomes even more pronounced in the study of nanomaterials and twodimensional materials. Systems such as graphene, silicene, germanene, stanene, phosphorene, MXenes, and various nanoribbon structures often require the use of large supercells to accurately describe atomic doping, defect formation, molecular adsorption, and surface interactions. As the system size increases, both the number of electronic states and the number of self-consistent field (SCF) iterations grow rapidly, leading to a substantial increase in computational cost. In many cases, a single geometry optimization or electronic structure calculation may require hundreds to thousands of processing cores operating continuously for hours or even days. Therefore, access to HPC resources has become a prerequisite for conducting advanced materials research with the accuracy required for predictive materials design and discovery [3].

Beyond ground-state calculations, HPC also enables the application of advanced methodologies that extend beyond conventional DFT, including DFT+U, hybrid exchange–correlation functionals, the GW approximation, the Bethe–Salpeter Equation (BSE), and Ab Initio Molecular Dynamics (AIMD). These approaches are typically tens to hundreds of times more computationally demanding than standard DFT calculations but provide significantly improved descriptions of electronic, optical, and excited-state properties. The combination of advanced quantum-mechanical methodologies with the computational power of HPC has facilitated the investigation of increasingly complex material systems and has substantially accelerated the discovery of novel materials for applications in electronics, energy technologies, catalysis, and quantum devices.

3.2. Molecular Dynamics Simulations

In addition to first-principles calculations, Molecular Dynamics (MD) simulations represent one of the most important areas of computational materials science and one of the most prominent applications of High-Performance Computing (HPC). The MD method describes the motion of atoms and molecules over time by solving Newton's equations of motion under the influence of interatomic forces. By tracking the trajectories of individual atoms, MD provides detailed insights into microscopic physical and chemical processes that are often difficult or impossible to observe directly through experimental techniques [14].

The advancement of HPC has enabled MD simulations to scale from systems containing a few thousand atoms to those involving millions or even billions of atoms. Widely used software packages such as LAMMPS, GROMACS, NAMD, and DL_POLY have been specifically designed for parallel computing environments, allowing material systems to be partitioned into independent computational domains and processed simultaneously across thousands of computational cores. Consequently, researchers can investigate physical phenomena occurring on timescales ranging from nanoseconds to microseconds or even longer, capabilities that are generally beyond the reach of conventional computing platforms [15–16].

In materials research, molecular dynamics simulations are extensively employed to study phasetransition phenomena such as melting, crystallization, recrystallization, and defect formation. MD also enables investigations of atomic diffusion, defect migration, heat transport mechanisms, and thermal stability under various temperature and pressure conditions. Particularly for nanomaterials and two-dimensional materials, MD plays a critical role in evaluating thermal robustness, structural stability, and material performance under realistic environmental conditions [17].

Furthermore, MD has become a powerful tool for studying adsorption and desorption processes involving atoms and molecules on material surfaces. Through time-dependent simulations, researchers can elucidate adsorption mechanisms, determine binding energies, identify diffusion pathways, and evaluate the stability of adsorbate–surface systems under different thermodynamic conditions. These capabilities are especially valuable in the development of gas-sensing materials, catalysts, energy-storage devices, and materials for hydrogen or carbon dioxide storage. In addition, MD simulations can be employed to investigate material–environment interactions, including corrosion, oxidation, and radiation-induced structural modifications [18].

Because MD simulations require the repeated calculation of interatomic forces and the continuous updating of atomic positions over millions of time steps, they demand substantial computational resources. Many state-of-the-art studies currently utilize thousands to tens of thousands of processing cores operating simultaneously on HPC systems for days or even weeks to simulate large-scale physical processes occurring over extended timescales. The emergence of petascale and exascale computing platforms continues to expand the capabilities of molecular dynamics simulations, enabling increasingly accurate multiscale investigations spanning from atomic-scale phenomena to microstructural evolution [3]. Consequently, HPC has become an indispensable foundation for modern MD research, contributing significantly to our understanding of material behavior and supporting the design of advanced materials for a wide range of technological applications.

3.3. Materials Discovery

One of the most remarkable achievements arising from the integration of High-Performance Computing (HPC) and modern materials science is the development of high-throughput computational materials discovery. Rather than relying solely on traditional trial-and-error experimental approaches, which are often time-consuming and costly, researchers can now employ HPC systems to perform millions of first-principles calculations for the screening, evaluation, and prediction of material properties prior to experimental synthesis. This paradigm has fundamentally transformed the methodology of materials research, significantly shortening the development cycle of new materials from years to months or, in some cases, even weeks [19].

The advancement of HPC infrastructures has facilitated the creation of large-scale materials databases based on automated Density Functional Theory (DFT) calculations. Representative examples include the Materials Project, the Open Quantum Materials Database (OQMD), and the AFLOW Consortium. These initiatives utilize millions of CPU-hours on supercomputing platforms to determine stable crystal structures, formation energies, band gaps, magnetic properties, mechanical strength, and numerous other important material characteristics. The resulting data are subsequently stored in open-access repositories, enabling researchers worldwide to access and exploit them for the discovery and design of novel materials [20–22].

Among these platforms, the Materials Project is recognized as one of the largest and most influential materials databases currently available. It employs standardized DFT calculations on HPC systems to establish a comprehensive repository containing hundreds of thousands of inorganic materials with consistently calculated structural and electronic properties. Similarly, OQMD was developed to provide formation energies and thermodynamic stability data for hundreds of thousands of inorganic compounds, thereby facilitating the prediction of previously unknown material phases. In contrast, the AFLOW Consortium focuses on automating firstprinciples computational workflows, enabling highly efficient large-scale materials screening campaigns on HPC platforms [21].

Thanks to the parallel processing capabilities of HPC systems, researchers can investigate tens of thousands to hundreds of thousands of material structures within a single computational campaign. This capability is particularly valuable for rapidly growing research areas such as lithium-ion and sodium-ion battery electrode materials, electrocatalysts, greenhouse gas adsorption materials, thermoelectric materials, photovoltaic materials, and quantum materials. In many cases, HPC enables the identification of promising candidate materials before any experimental evidence becomes available, thereby substantially reducing research costs and accelerating technological innovation. More recently, the integration of HPC with artificial intelligence (AI) and machine learning (ML) has introduced a new paradigm for materials discovery. Databases generated from millions of DFT calculations performed on HPC systems provide extensive training datasets for machine learning models capable of predicting material properties at speeds far exceeding those of conventional quantum-mechanical calculations. The convergence of HPC, DFT, and AI is expected to further advance the concept of materials by design and contribute to addressing critical challenges in energy, environmental sustainability, and next-generation electronic technologies [22].

3.4. Simulation of Nanomaterials and Two-Dimensional Materials

The discovery of graphene in 2004 opened an entirely new frontier in the field of nanomaterials and two-dimensional (2D) materials. Since then, a broad range of atomically thin materials, including silicene, germanene, stanene, phosphorene, borophene, MXenes, and van der Waals heterostructures, have attracted considerable attention owing to their exceptional electronic, magnetic, mechanical, and optical properties. These materials are regarded as highly promising candidates for next-generation electronic devices, gas sensors, energy storage systems, spintronic applications, and quantum technologies. However, accurately investigating their properties requires substantial computational resources because of the complexity of their electronic structures and the sensitivity of their physical properties to atomic-scale modifications [23–24].

In nanomaterials research, phenomena such as atomic doping, gas adsorption, lattice defects, mechanical strain, structural phase transitions, and spin-related effects play critical roles in tailoring material properties. To accurately describe these processes, computational models typically employ large supercells to minimize artificial interactions arising from periodic boundary conditions. Furthermore, the investigation of electronic structures in two-dimensional materials requires dense k-point sampling within the Brillouin zone to ensure the convergence of physical quantities such as total energy, density of states (DOS), and electronic band structures. As model sizes increase, computational costs rise rapidly, making HPC resources indispensable for modern materials research [25].

In studies involving atomic doping, HPC enables the simultaneous exploration of multiple substitutional or adsorption sites to identify the most stable configurations. For materials such as silicene, germanene, and stanene nanoribbons, doping with transition metals or main-group elements can significantly alter band gaps, magnetic moments, and electronic transport properties. Comprehensive investigations of these effects often require dozens or even hundreds of structural optimizations and self-consistent electronic calculations, demanding substantial HPC resources [26].

Gas adsorption on nanomaterials represents another important research direction for the development of highly sensitive gas sensors and advanced energy storage materials. Molecules such as CO, CO_2, NO, NO_2, NH_3, H_2, and H_2S are frequently investigated on graphene, stanene, silicene, and MXene surfaces through large-scale DFT calculations. Determining adsorption energies, charge transfer mechanisms, density of states, and molecule–surface interactions requires extensive calculations involving multiple adsorption configurations. HPC significantly reduces computational time and enables the rapid screening of numerous material systems for sensing and catalytic applications [27–28].

Beyond doping and adsorption studies, HPC also plays a crucial role in exploring advanced quantum phenomena such as spin–orbit coupling, spin polarization, the quantum Hall effect, and topological states in two-dimensional materials. These phenomena often require computationally demanding approaches, including DFT+U, hybrid functionals, GW calculations, and the Bethe– Salpeter equation (BSE), which are substantially more expensive than conventional DFT methods. Through large-scale parallel processing across thousands of computational cores, HPC facilitates in-depth investigations of emerging quantum materials and supports the development of future nanoelectronic and spintronic devices [3].

Overall, the integration of HPC with advanced quantum-mechanical simulation techniques has enabled unprecedented investigations of nanomaterials and two-dimensional materials. This capability not only deepens our understanding of fundamental physical mechanisms but also provides an efficient pathway for designing novel materials for next-generation electronic, energy, and quantum technologies.

3.5. Integration of HPC and Artificial Intelligence in Materials Discovery

In recent years, the convergence of High-Performance Computing (HPC), Artificial Intelligence (AI), and data science has emerged as one of the most significant developments in modern materials research. The rapid advancement of HPC infrastructures has enabled millions of firstprinciples calculations, molecular dynamics (MD) simulations, and multiscale modeling studies, generating an unprecedented volume of materials data. These datasets contain valuable information on crystal structures, formation energies, band gaps, electronic densities of states, mechanical strength, magnetic properties, electrical conductivity, and catalytic activities for hundreds of thousands to millions of compounds. However, effectively extracting knowledge from such massive datasets requires advanced analytical and predictive tools that go far beyond conventional statistical approaches. In this context, AI and Machine Learning (ML) have become ideal companions to HPC, accelerating the discovery and rational design of novel materials [29].

Machine learning models are capable of learning from datasets generated through DFT and MD simulations performed on HPC platforms, thereby establishing complex relationships between material structures and their corresponding physical or chemical properties. Once trained, these models can predict a wide range of important quantities, including band-gap energies, formation energies, mechanical strength, electrical conductivity, thermal conductivity, thermodynamic stability, and catalytic activity, at speeds that are thousands to millions of times faster than traditional quantum-mechanical calculations. This capability significantly reduces computational costs and enables the rapid screening of vast numbers of candidate materials before more accurate simulations or experimental validations are conducted [30].

One of the key factors driving the application of AI in materials science is the emergence of largescale materials databases such as Materials Project, Open Quantum Materials Database (OQMD), AFLOW, and NOMAD. These repositories have been constructed using millions of DFT calculations performed on HPC systems and currently contain information on hundreds of thousands of material structures. Such extensive datasets serve as valuable training resources for modern machine learning algorithms, improving prediction accuracy and expanding the applicability of AI-driven approaches in materials research [31–32].

The integration of HPC and AI has given rise to a new research discipline known as Materials Informatics. The primary objective of this field is to exploit large-scale materials data to develop predictive models capable of enabling “materials by design.” Rather than investigating individual materials through computationally expensive quantum-mechanical calculations, researchers can employ AI models to screen millions of candidate materials within a short period of time and subsequently select only the most promising structures for detailed DFT calculations or experimental validation. This strategy has already been successfully applied to the development of lithium-ion battery materials, electrocatalysts, thermoelectric materials, photovoltaic materials, and next-generation quantum materials [33].

Looking forward, the combination of exascale HPC systems with advanced deep learning algorithms, graph neural networks, and foundation models for materials science is expected to further accelerate the transition from trial-and-error materials discovery toward data-driven materials design. The convergence of HPC, AI, and quantum simulations will not only enhance research efficiency but also enable the discovery of entirely new classes of materials capable of addressing major challenges in energy, environmental sustainability, electronics, and quantum technologies. Consequently, HPC and AI are increasingly recognized as two foundational technological pillars that will shape the future of materials science in the digital era.

4. COMMON MATERIALS SIMULATION SOFTWARE ON HPC PLATFORMS

The rapid advancement of high-performance computing (HPC) systems has driven the development and refinement of a wide range of specialized materials simulation software packages. These software tools are built upon advanced computational methodologies, including Density Functional Theory (DFT), Molecular Dynamics (MD), Ab Initio Molecular Dynamics (AIMD), Non-Equilibrium Green's Function (NEGF) theory, and multiscale modeling approaches, enabling the investigation of material properties from the atomic to the mesoscale level. By effectively exploiting the massively parallel architectures of modern HPC systems, these software packages can perform computationally intensive calculations that would be impractical on conventional computing platforms.

Among DFT-based materials simulation packages, the Vienna Ab initio Simulation Package (VASP) is widely regarded as one of the most reliable and extensively used tools in computational materials science. VASP employs a plane-wave basis set combined with the projector augmentedwave (PAW) method to solve the Kohn–Sham equations, enabling the study of electronic structures, band structures, density of states, optical properties, magnetic properties, and ab initio molecular dynamics. Owing to its efficient parallel scalability across thousands of processing cores, VASP has become a standard tool in advanced materials research, particularly for nanomaterials and two-dimensional materials [11,34].

In addition to VASP, Quantum ESPRESSO is one of the most widely adopted open-source software suites within the materials science community. This package provides a comprehensive set of tools based on DFT and Density Functional Perturbation Theory (DFPT), supporting investigations of electronic structures, lattice vibrations, electron–phonon interactions, and optical properties. Thanks to its excellent scalability on HPC systems, Quantum ESPRESSO is extensively utilized in both academic research and large-scale materials database projects worldwide [35–36].

CASTEP and ABINIT are also important DFT-based software packages in computational materials science. CASTEP is developed using plane-wave basis sets and ultrasoft pseudopotentials, enabling accurate studies of electronic, optical, and vibrational properties of a wide range of materials. Meanwhile, ABINIT is a powerful open-source platform that supports calculations of electronic structures, phonons, dielectric properties, and excited-state phenomena. Both software packages have been optimized for HPC environments and are widely employed in high-accuracy materials simulations [37–38].

For large-scale materials systems containing hundreds or thousands of atoms, SIESTA offers an efficient alternative by employing localized atomic orbital basis sets rather than plane waves. This approach substantially reduces computational cost and memory requirements, making it particularly suitable for studying large nanoscale systems such as nanoribbons, amorphous materials, and complex defect structures. Due to its favorable scalability on HPC architectures, SIESTA has been extensively applied in research on two-dimensional materials and biomaterials [39].

In the field of molecular dynamics simulations, LAMMPS and GROMACS are among the most widely used software packages on HPC platforms. LAMMPS is specifically designed for largescale simulations of metals, ceramics, polymers, and nanomaterials, with the capability of handling millions of atoms across thousands of computational cores. In contrast, GROMACS is particularly renowned for biomolecular simulations, soft matter studies, and computational chemistry applications due to its exceptional performance on modern CPU and GPU architectures [40–41].

Furthermore, CP2K is a powerful software package for ab initio molecular dynamics and quantum chemistry simulations. It integrates DFT-based electronic structure calculations with molecular dynamics to investigate realistic processes such as chemical reactions, surface interactions, and energy materials phenomena. Through its efficient utilization of modern HPC resources, CP2K has become an important tool in catalysis and electrochemical materials research [42].

For nanoscale electronic transport studies, nanoDCAL represents a specialized computational platform that combines DFT with the Non-Equilibrium Green's Function (NEGF) formalism. This software enables the investigation of electronic transport properties, quantum current flow, transmission spectra, and device characteristics at the atomic scale. nanoDCAL has been widely applied to studies of nanoribbons, two-dimensional materials, and next-generation nanoelectronic devices [43–44].

Overall, modern materials simulation software has been continuously developed and optimized for HPC environments through advanced parallelization techniques based on MPI, OpenMP, and GPU computing. The synergy between state-of-the-art quantum mechanical algorithms and HPC infrastructures has enabled increasingly accurate simulations of complex material systems, thereby accelerating the discovery and design of novel materials for a broad range of scientific and technological applications.

5. CHALLENGES AND FUTURE DEVELOPMENT TRENDS OF HPC IN MATERIALS SIMULATION

Although high-performance computing (HPC) systems have brought remarkable advances to the field of materials simulation, the effective utilization of these platforms still faces numerous technical and economic challenges. As the scale of simulations continues to expand and the accuracy requirements of computational methods become increasingly stringent, the demand for computational resources, energy consumption, and hardware infrastructure grows substantially. Consequently, new requirements are emerging for the development of next-generation HPC systems capable of meeting the rapidly increasing demands of the materials science community [45].

One of the most significant challenges is the enormous energy consumption of modern supercomputers. Petascale and exascale systems may comprise millions of processing cores and tens of thousands of GPU accelerators operating simultaneously, resulting in power consumption levels reaching tens of megawatts. As a consequence, the costs associated with operation, cooling, and maintenance of HPC data centers continue to rise. In the context of global efforts toward sustainable development and carbon emission reduction, improving the energy efficiency of HPC systems has become a major objective of the supercomputing industry [46–47].

In addition to energy-related concerns, the deployment and maintenance of HPC infrastructures require substantial financial investments. The costs of computing hardware, high-speed networking, large-scale data storage systems, and specialized software can reach hundreds of millions of dollars for leading supercomputing facilities worldwide. Furthermore, the efficient operation of these systems requires highly skilled personnel with expertise in computer architecture, parallel programming, algorithm optimization, and system administration. These requirements constitute significant barriers for many research institutions and universities, particularly in developing countries [3].

Another important technical challenge lies in the scalability of materials simulation algorithms on modern HPC architectures. Advanced quantum-mechanical approaches, including hybrid functionals, the GW approximation, the Bethe–Salpeter equation (BSE), and strongly correlated electronic structure methods, often involve extremely high computational complexity and do not scale efficiently across hundreds of thousands or even millions of processing cores. Consequently, the development of novel algorithms capable of fully exploiting the parallel capabilities of exascale systems has become a critical research direction in computational materials science [30].

Looking ahead, the emergence of exascale computing is expected to initiate a new era in materials simulation. Exascale supercomputers, capable of performing more than 10^18 floating-point operations per second, will enable the investigation of materials systems far larger and more complex than those currently accessible. These systems will also facilitate simulations of physical phenomena occurring across multiple spatial and temporal scales. At the same time, nextgeneration GPU accelerators equipped with tens of thousands of parallel computing cores are becoming central components of modern HPC architectures, significantly enhancing computational performance while reducing energy consumption per calculation [8].

Another particularly important trend is the integration of HPC with artificial intelligence (AI). Deep learning algorithms, graph neural networks, and foundation models for materials science are increasingly being employed to replace or complement computationally demanding quantummechanical calculations. Within this emerging research paradigm, HPC serves not only as a platform for large-scale DFT and molecular dynamics simulations but also as the computational backbone for training AI models containing billions of parameters. The synergy between HPC and AI is expected to dramatically accelerate the discovery of novel materials while extending computational investigations to systems that are beyond the practical reach of conventional approaches [29–30].

In addition, quantum computing is emerging as a promising technology that may complement HPC in the future. Although quantum computing remains at an early stage of development, growing evidence suggests that the integration of HPC with quantum processors could provide powerful solutions for many-body quantum problems, strongly correlated electronic systems, and other complex materials challenges that remain difficult for classical computational methods. Hybrid quantum–classical computing frameworks are therefore regarded as a highly promising approach for combining the strengths of traditional HPC platforms with the unique capabilities of quantum computing [48].

Overall, despite persistent challenges related to energy consumption, infrastructure costs, and algorithm scalability, HPC continues to play a central role in modern materials research. The continued advancement of exascale systems, next-generation GPUs, artificial intelligence, and quantum computing is expected to create a more powerful computational ecosystem capable of addressing increasingly complex materials science problems and accelerating the realization of data-driven materials design in the future.

6. CONCLUSION

High-performance computing (HPC) has become a fundamental infrastructure underpinning modern materials research. From density functional theory (DFT) calculations and molecular dynamics simulations to high-throughput materials discovery and the integration of artificial intelligence, HPC plays a pivotal role in accelerating scientific investigations, reducing experimental costs, and improving the accuracy and reliability of theoretical predictions. The unprecedented computational power provided by HPC has enabled researchers to explore increasingly complex material systems across multiple spatial and temporal scales, thereby significantly advancing the understanding of structure–property relationships and facilitating the rational design of novel materials. As data-driven science, artificial intelligence, and advanced computational technologies continue to evolve, HPC is expected to play an even more critical role in the future of materials science. The convergence of exascale computing, machine learning, and next-generation simulation methodologies will further enhance the capability to predict, screen, and optimize materials with unprecedented efficiency. Consequently, HPC will remain an indispensable tool for the design and development of advanced materials, supporting technological innovations in energy, electronics, quantum technologies, environmental sustainability, and other key areas of future scientific and industrial advancement.

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