

Review

Emerging Frontiers in Computational Physics: From DFT to AI-Assisted Modeling

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DOI: 10.62896/ijmsi.2.s1.02

Conflict of interest: NIL

Article History

Received: 08/06/2026

Accepted: 16/06/2026

Published: 20/06/2026

Abstract:

Computational physics has traversed a remarkable journey over the past five decades, evolving from rudimentary numerical methods to highly sophisticated quantum-mechanical simulations. The discipline today occupies a central position in both fundamental research and applied materials science. Density functional theory (DFT) provided the first practical framework for solving the many-body electron problem with acceptable computational cost, and its widespread adoption transformed how researchers study electronic structure, bonding, and material properties. In recent years, machine learning and artificial intelligence have begun reshaping this landscape once more, enabling models that combine the accuracy of quantum mechanics with computational speeds that were previously unimaginable. This review surveys the historical development of computational physics methods, examines landmark contributions that defined each era, and assesses the current state of AI-assisted modeling. Particular attention is paid to the integration of neural network interatomic potentials, generative models for materials discovery, and physics-informed neural networks. Challenges associated with transferability, interpretability, and data quality are discussed, along with an assessment of the most promising directions for future research.

Keywords: computational physics, density functional theory, machine learning potentials, neural network force fields, physics-informed neural networks, materials discovery.

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I. INTRODUCTION

The capacity to predict the physical and chemical behavior of matter from first principles has long stood as one of the most ambitious objectives in science. Computational physics, broadly defined as the use of algorithms and numerical methods to solve physical problems that resist analytical treatment, has steadily narrowed the gap between theoretical conjecture and experimental verification. From the earliest Monte Carlo simulations of hard-sphere fluids conducted by Metropolis and colleagues at Los Alamos in 1953 [1] to the petascale molecular dynamics runs of today, each computational advance has opened new windows onto phenomena previously inaccessible to direct measurement.

The field was transformed irrevocably with the formulation of density functional theory by Walter Kohn and Lu Jeu Sham in 1965 [2], building upon the earlier Hohenberg-Kohn theorems [3]. DFT recast the intractable N-electron Schrödinger equation into a set of single-particle equations governed by an effective potential, making ground-state calculations of real materials genuinely feasible. Over the following decades, the development of exchange-correlation functionals, pseudopotentials, and plane-wave basis sets extended DFT into a workhorse that now underpins thousands of publications annually across chemistry, condensed matter physics, and materials engineering.

Despite these successes, DFT carries well-documented limitations. The local density approximation and many generalized-gradient approximations underestimate band gaps in semiconductors and insulators, describe van der Waals interactions poorly, and struggle with strongly correlated electron systems such as Mott insulators and heavy-fermion compounds. Post-DFT methods including DFT+U, hybrid functionals, GW approximation, and dynamical mean-field theory have each addressed a subset of these deficiencies at the cost of increased computational burden. The practical ceiling of routine DFT calculations thus remained at system sizes of a few hundred atoms for ab initio molecular dynamics, leaving mesoscale and macroscale phenomena out of reach.

The entry of machine learning into computational physics, accelerated after the pioneering work of Behler and Parrinello on neural network potentials in 2007 [4], has begun breaking through this ceiling. By training flexible models on DFT-generated datasets, researchers can now run molecular dynamics simulations at near-DFT accuracy while achieving computational throughputs comparable to classical force fields, which are orders of magnitude faster. More recently, architectures such as graph neural networks, equivariant message-passing networks, and transformer-based models have pushed the accuracy frontier further while enabling transferability across diverse chemical environments. Simultaneously, generative artificial intelligence is beginning to assist in the inverse design of materials, suggesting stable structures with targeted properties before any experiment is performed.

This review is organized as follows. Section II surveys the foundational quantum mechanical methods that gave computational physics its analytical backbone. Section III examines the development and current status of DFT and its principal extensions. Section IV discusses classical and reactive force fields as the intermediate link between quantum and continuum methods. Section V details the emergence of machine learning interatomic potentials and their landmark applications. Section VI addresses physics-informed neural networks and equation-discovery approaches. Section VII discusses AI-assisted materials discovery and high-throughput screening. Section VIII outlines outstanding challenges, and Section IX concludes with a perspective on future directions.

II. QUANTUM MECHANICAL FOUNDATIONS

Long before DFT arrived, the variational principle and the Hartree-Fock (HF) approximation provided the primary language of electronic structure. Hartree introduced self-consistent field equations in 1928 [5], and Fock's antisymmetrized extension a year later placed these equations on a rigorous many-body footing. HF theory correctly captures exchange effects but neglects electronic correlation entirely, a deficiency measured by the correlation energy, which is defined as the difference between the exact nonrelativistic ground-state energy and the HF limit. For many molecular systems, this correlation energy amounts to a chemically significant fraction of a few tens of kilocalories per mole.

Møller-Plesset perturbation theory [6], configuration interaction, and coupled cluster methods progressively recovered correlation at the expense of steep polynomial scaling with system size. The gold standard of quantum chemistry, coupled cluster with singles, doubles, and perturbative triples (CCSD(T)), achieves sub-kilojoule accuracy for small molecules but scales formally as $O(N^7)$ with the number of electrons, confining its practical application to systems of fewer than a few dozen atoms. Quantum Monte Carlo methods, particularly diffusion Monte Carlo, offer an alternative stochastic route to correlated many-body wave functions and have achieved remarkable accuracy for benchmark systems including solid hydrogen under extreme pressure [7], but they too remain computationally demanding.

The many-body perturbation theory framework provided by Hedin's GW approximation [8] addressed the quasiparticle band gap problem that afflicts DFT, and its implementation in codes such as BerkeleyGW and ABINIT enabled the accurate prediction of photoemission and optical spectra for semiconductors and insulators. Bethe-Salpeter equation calculations built on top of GW results further enabled the quantitative simulation of excitonic optical absorption, which is critical for photovoltaic and optoelectronic applications. These methods, while computationally expensive, established reliable benchmarks against which lighter approximations are validated.

III. DENSITY FUNCTIONAL THEORY AND ITS EXTENSIONS

The Hohenberg-Kohn theorem establishes that the ground-state energy of an interacting electron gas in an external potential is a unique functional of the electron density alone [3]. This deceptively simple statement, together with

the Kohn-Sham ansatz that replaces the interacting system with a fictitious noninteracting system reproducing the same density [2], converted an exponentially complex problem into one solvable in polynomial time. The only quantity requiring approximation is the exchange-correlation energy functional, and decades of effort have produced a hierarchical sequence of approximations, famously organized by Perdew into Jacob's ladder.

The local density approximation, derived from the uniform electron gas, served as the workhorse of early DFT calculations and continues to be used for solids where electron densities are nearly uniform. The generalized gradient approximation, and in particular the PBE functional of Perdew, Burke, and Ernzerhof [9], corrected several of LDA's systematic errors and became the de facto standard for solid-state calculations after its publication in 1996. Its widespread adoption was facilitated by efficient implementations in codes such as VASP, Quantum ESPRESSO, and WIEN2k, which remain among the most heavily cited software packages in all of computational science.

Hybrid functionals, which incorporate a fraction of exact HF exchange, were introduced by Becke in 1993 [10] and later tuned into the highly successful HSE06 functional by Heyd, Scuseria, and Ernzerhof. Hybrid functionals corrected the band-gap underestimation that plagued LDA and GGA and enabled quantitative predictions of electronic properties for semiconductors including silicon, germanium, and gallium arsenide with unprecedented fidelity. For magnetic insulators and transition metal oxides, the DFT+U approach introduced by Anisimov and colleagues [11] added a Hubbard-like on-site Coulomb interaction to localized d and f electrons, partially restoring the correct Mott-insulator description. Landmark studies on iron oxide, nickel oxide, and the cuprate superconductors validated this approach against experimental spectroscopy.

Dispersion-corrected DFT methods, most notably the DFT-D3 correction by Grimme and collaborators [12] and the many-body dispersion approach by Tkatchenko and Scheffler [13], addressed the longstanding failure of standard functionals to capture non-covalent interactions. These corrections proved indispensable for modeling molecular crystals, layered materials including graphene and transition metal dichalcogenides, and host-guest binding in metal-organic frameworks. More recently, meta-GGA functionals such as SCAN (strongly

constrained and appropriately normed) developed by Sun, Ruzsinszky, and Perdew [14] have demonstrated superior accuracy across a broad range of bonding environments while satisfying all known exact constraints of the exchange-correlation functional, representing a significant conceptual and practical advance over PBE.

Ab initio molecular dynamics, introduced by Car and Parrinello in 1985 [15] in a landmark paper that fused DFT with classical equations of motion through a fictitious electron mass, allowed finite-temperature dynamics to be propagated at quantum mechanical accuracy. The Car-Parrinello method and its Born-Oppenheimer molecular dynamics successors enabled the study of liquid water, aqueous chemistry, phase transitions, and thermodynamic properties of minerals under geophysically relevant conditions. Extensions combining DFT with non-equilibrium Green's functions, introduced by Landauer, Büttiker, and later implemented computationally by Brandbyge and collaborators [16], opened the field of computational nanoelectronics, enabling quantitative prediction of electron transport through single molecules and nanoscale devices.

IV. CLASSICAL AND REACTIVE INTERATOMIC POTENTIALS

Classical molecular dynamics and Monte Carlo methods, which operate on empirically parameterized potential energy surfaces rather than solving the Schrödinger equation, extended the accessible system sizes to millions of atoms and timescales to microseconds and beyond. Pair potentials such as Lennard-Jones and Buckingham forms captured the essential physics of noble gas systems and ionic crystals but failed for metals and covalent semiconductors. Embedded atom method potentials developed by Daw and Baskes [17] incorporated many-body effects through an embedding energy that depends on the local electron density, enabling realistic simulations of metallic systems including crack propagation, grain boundary diffusion, and surface reconstruction.

Reactive force fields represented a further advance by allowing bond formation and breaking to be modeled without quantum mechanics. The ReaxFF framework developed by van Duin and Goddard [18] parameterized bond-order-dependent potentials against quantum chemical data and found wide application in combustion chemistry, corrosion, and heterogeneous catalysis. The Tersoff potential [19] and the Stillinger-Weber potential [20] addressed covalent materials such as silicon and

germanium, reproducing bulk elastic constants and melting points with reasonable accuracy. While these empirical potentials enabled simulations of unprecedented scale, their accuracy remained limited by the functional forms assumed and their inability to adapt to chemical environments outside the training set.

V. MACHINE LEARNING INTERATOMIC POTENTIALS

The pivotal insight underlying machine learning potentials is that the total energy of a system can be decomposed into atomic contributions, each depending on the local chemical environment described by a set of symmetry-invariant descriptor functions. Behler and Parrinello introduced this framework in 2007 [4], using atom-centered symmetry functions as descriptors and feed-forward neural networks as function approximators. The resulting high-dimensional neural network potential (HDNNP) reproduced the DFT energy surface for bulk copper with root mean square errors below one millielectronvolt per atom while enabling molecular dynamics runs at orders-of-magnitude lower cost.

The Gaussian approximation potential (GAP) framework developed by Csányi and collaborators [21] took a non-parametric Gaussian process regression approach, representing the potential energy surface as a sum of kernel functions evaluated against a database of reference configurations. The SOAP (smooth overlap of atomic positions) descriptor developed alongside GAP proved particularly effective at capturing local environment similarity and has since been adopted broadly in the machine learning potential community. Applications to liquid water, amorphous carbon, and tungsten under irradiation demonstrated that GAP potentials could reach near-DFT accuracy for systems where no classical force field existed.

Graph neural network potentials transformed the field by operating directly on the atomic graph rather than on hand-crafted descriptor vectors. The SchNet architecture introduced by Schütt and collaborators [22] used continuous-filter convolutional networks to learn rotationally invariant feature representations from atom positions and atomic numbers. DimeNet, PaiNN, and subsequent architectures incorporated angular information and equivariant representations, further improving accuracy and transferability. The equivariant message-passing framework underlying NequIP, developed by Batzner and collaborators [23], and the MACE architecture

by Batatia and colleagues [24] established new accuracy benchmarks on standard datasets including MD17, QM9, and the Open Catalyst Project, approaching CCSD(T) quality on molecular test sets.

The FLARE framework by Vandermause and collaborators extended the Bayesian uncertainty quantification approach of GAP into an on-the-fly active learning scheme [25]. By estimating prediction uncertainty during molecular dynamics, FLARE triggered DFT calculations only when the model encountered unfamiliar configurations, autonomously expanding the training set and eliminating the laborious manual curation that previously bottlenecked potential development. This active learning paradigm was subsequently implemented in various flavors across DeePMD [26], ACE, and M3GNet potentials, substantially reducing the human effort required to build transferable models for complex multi-component systems.

The DeePMD-kit framework developed by Zhang and collaborators [26] enabled large-scale molecular dynamics with deep potential molecular dynamics (DPMD) models trained by end-to-end deep learning and implemented with GPU acceleration. Simulations of liquid water at 192,000 atoms for nanosecond timescales, combined with free energy perturbation methods, yielded radial distribution functions and diffusion coefficients in quantitative agreement with experiment. A particularly striking demonstration came from studies of the phase diagram of water under megabar pressures, directly relevant to planetary science, where DFT-quality accuracy would have been computationally prohibitive without the DPMD approach.

Foundation models for atomistic simulation represent the most recent frontier in machine learning potentials. MACE-MP-0, trained by Batatia and collaborators on the MPTrj dataset derived from the Materials Project database, demonstrated zero-shot transferability across 89 elements and diverse bonding environments without any system-specific fine-tuning [24]. The ALIGNN-FF model and the CHGNet universal potential similarly pursued broad coverage of the periodic table. These universal potentials, while not yet matching bespoke models in accuracy for specific systems, have dramatically lowered the barrier to rapid computational screening and are increasingly used as starting points for fine-tuning on targeted applications.

VI. PHYSICS-INFORMED NEURAL NETWORKS AND EQUATION DISCOVERY

A parallel strand of AI integration into computational physics developed around the idea of encoding physical laws directly into the architecture and loss function of neural networks, rather than treating them as a black box trained exclusively on data. Raissi, Perdikaris, and Karniadakis introduced physics-informed neural networks (PINNs) in 2019 [27], demonstrating that partial differential equations governing fluid flow, heat transfer, and wave propagation could be solved by minimizing a composite loss function that penalized both deviations from boundary and initial conditions and violations of the governing equations evaluated at collocation points. Unlike conventional numerical methods, PINNs require no spatial mesh and can naturally handle inverse problems in which some parameters of the governing equations are unknown.

Applications of PINNs to computational physics have expanded rapidly. In quantum mechanics, PINNs have been used to solve the Schrödinger equation for anharmonic oscillators and multi-electron atoms, recovering ground and excited state wave functions without discretizing the Hilbert space. In plasma physics, PINNs have been applied to the Vlasov equation describing phase-space distribution functions in fusion plasmas, offering potential advantages in adaptive refinement of phase-space grids. In solid mechanics, PINN-based surrogate models for stress and strain fields in heterogeneous microstructures have been used to accelerate finite-element calculations for materials with complex geometries.

Data-driven discovery of governing equations represents a related but distinct objective. The sparse identification of nonlinear dynamics (SINDy) algorithm introduced by Brunton, Proctor, and Kutz [28] constructed libraries of candidate terms and used sparse regression to identify the minimal set of terms consistent with time-series data, successfully recovering equations of motion for chaotic systems including the Lorenz attractor and the nonlinear pendulum from noisy measurement data. Extensions of SINDy to partial differential equations, applied to experimental fluid dynamics data, recovered the Navier-Stokes equations directly from velocity field measurements, demonstrating a path toward physics discovery that does not presuppose the governing equations.

The neural operator framework, encompassing the Fourier neural operator (FNO) introduced by Li and collaborators

[29] and its successor the geometry-informed neural operator (GINO), advanced the idea of learning mappings between function spaces rather than input-output pairs. FNOs operate in Fourier space to capture long-range correlations efficiently and have demonstrated three orders of magnitude speedup over conventional finite element solvers for turbulent flow problems while preserving sub-percent relative errors. These operators are mesh-independent and can generalize across different resolutions, a property that conventional neural networks lack and that makes them particularly valuable as surrogate models in high-throughput computational workflows.

VII. AI-ASSISTED MATERIALS DISCOVERY AND HIGH-THROUGHPUT SCREENING

The convergence of high-throughput DFT, materials databases, and machine learning has created a new paradigm for computational materials discovery that operates at a scale impossible with human-directed research alone. The Materials Project, launched by Jain, Ong, and Hautier in collaboration with Ceder and Persson, assembled DFT-computed properties for over 150,000 inorganic compounds and provided an open application programming interface enabling programmatic queries [30]. The AFLOW database, the OQMD, and the NOMAD repository similarly accumulated tens of thousands of calculated band structures, elastic tensors, and formation energies, forming the raw material from which machine learning models could extract composition-property relationships.

Crystal structure prediction has been a particularly active area of AI-assisted research. The random structure searching method developed by Pickard and Needs [31] combined with metadynamics, evolutionary algorithms, and more recently machine learning energy landscapes has identified high-pressure phases of hydrogen, lithium, and boron hydrides with superconducting transition temperatures that were subsequently confirmed experimentally. The CALYPSO and USPEX codes automated evolutionary crystal structure search guided by first-principles calculations and discovered novel phases of carbon, nitrogen, and binary intermetallics that challenge conventional bonding intuitions.

Generative models for inorganic crystal structures represent the most recent entrant in this area. Crystal Diffusion Variational Autoencoder (CDVAE) introduced by Xie and collaborators [32] learned to generate stable crystal structures by operating in a latent space regularized

by physical constraints including charge neutrality and stoichiometric validity. DiffCSP and FlowMM extended these ideas using diffusion models and continuous normalizing flows, respectively, achieving higher diversity and structural validity rates than earlier variational approaches. These models are beginning to be applied to inverse design tasks in which the user specifies a target property such as a band gap or ionic conductivity and the model proposes candidate structures likely to possess that property.

Property prediction from composition and structure using graph neural networks has become sufficiently reliable for industrial screening workflows. CGCNN [33], developed by Xie and Grossman, was among the first to represent crystal structures as multi-edge graphs and demonstrated accurate prediction of formation energies, band gaps, and elastic moduli across diverse compound classes. MEGNet by Chen and collaborators, and later the M3GNet and CHGNet architectures, improved upon CGCNN by incorporating global state information, spin and magnetic moment predictions, and uncertainty quantification through ensemble or Bayesian approaches. Pharmaceutical companies and battery materials startups have begun deploying variants of these models in commercial screening pipelines, reflecting the transition of AI-assisted computation from academic curiosity to industrial tool.

Large language models and multimodal foundation models are beginning to make inroads into materials science in a different way, serving as interfaces between natural-language scientific literature and structured materials databases. Models such as MatBERT and MatSciBERT [34], pre-trained on corpora of materials science papers, demonstrated state-of-the-art performance on named entity recognition, relation extraction, and information retrieval tasks relevant to experimental synthesis conditions, dopant concentrations, and processing parameters. These models, when coupled to databases and DFT engines, offer a path toward fully automated literature-to-simulation pipelines, though questions about hallucination and factual reliability remain significant obstacles in safety-critical applications.

VIII. CHALLENGES AND OPEN QUESTIONS

Despite remarkable progress, several fundamental challenges continue to limit the scope and reliability of AI-assisted computational physics. Transferability remains the central concern for machine learning potentials: models trained on equilibrium and near-equilibrium configurations may fail catastrophically for rare events such as chemical

reactions, phase transitions, and surface reconstructions that involve configurations far from the training distribution. Uncertainty quantification methods including committee models, Bayesian neural networks, and conformal prediction offer partial remedies by flagging extrapolation, but reliable uncertainty estimates in high-dimensional configuration spaces remain an active and unsolved research problem.

The interpretability of neural network models presents a further challenge for physics. Classical force fields and even DFT calculations admit physical interpretations in terms of bond orders, partial charges, and orbital hybridization. Deep neural networks, by contrast, distribute information across millions of parameters in ways that resist simple physical interpretation. Efforts toward explainable AI in materials science, including attention visualization in graph networks, gradient-based feature attribution methods, and symbolic regression applied to learned representations, are beginning to extract physically meaningful patterns but have not yet achieved the interpretive clarity that experimental or classical theoretical methods provide.

Data quality and diversity present practical bottlenecks for model training. DFT calculations themselves carry systematic errors from the choice of exchange-correlation functional, and those errors propagate into any model trained on DFT data. When machine learning models are trained on PBE-GGA data and applied to systems where PBE fails, for example correlated oxides or charge-transfer molecular crystals, the accuracy ceiling imposed by the training data limits the utility of even the most sophisticated architecture. Addressing this requires either higher-level reference data, which is expensive to generate, or physics-based corrections that bridge levels of theory, an active area of research under the umbrella of transfer learning and delta machine learning.

Timescale and length scale limitations, while substantially relaxed by machine learning potentials relative to DFT, have not been eliminated. Rare events including nucleation, diffusion of defects, and conformational transitions in biomolecules occur on timescales of microseconds to seconds that remain inaccessible even to the fastest ML-MD simulations without enhanced sampling techniques. Methods including metadynamics, replica exchange, and variational approaches to the committor function are being integrated with machine learning force fields, and this integration is likely to yield

significant advances in the simulation of long-timescale processes within the next decade.

IX. FUTURE DIRECTIONS

The next generation of computational physics will likely be characterized by increasingly seamless integration across scales and methods. Multiscale frameworks that pass information from quantum mechanical calculations to machine learning potentials, and from atomistic simulations to continuum models, are being assembled into automated workflows by projects including AiiDA, FireWorks, and Atomate2. These workflow managers, combined with high-performance computing clusters and cloud resources, are enabling truly high-throughput explorations of compositional and structural space that were inconceivable a decade ago.

Quantum computing represents a longer-term but potentially transformative addition to the computational physicist's toolkit. Variational quantum eigensolver (VQE) algorithms implemented on near-term noisy intermediate-scale quantum (NISQ) devices have demonstrated proofs of concept for small molecular systems including hydrogen and lithium hydride. Fault-tolerant quantum algorithms, particularly the phase estimation algorithm, are projected to provide exponential speedups over classical methods for strongly correlated electron problems once sufficiently large and coherent quantum processors become available, a transition that most experts estimate to be at least one to two decades away.

The integration of generative AI with autonomous laboratory systems, sometimes described as self-driving laboratories, may prove transformative for closing the loop between computation and experiment. Robotic synthesis platforms at institutions including the University of Toronto, MIT, and Carnegie Mellon University have demonstrated autonomous material synthesis and characterization directed by Bayesian optimization algorithms. When coupled to fast ML-surrogate models rather than slow DFT calculations, these systems can in principle traverse material space at rates that no human-directed research program can match. Early demonstrations in polymer electrolyte design, photocatalyst optimization, and thin-film solar cell fabrication have validated the feasibility of this approach.

It would be an overstatement to suggest that artificial intelligence will replace the physicist's intuition and analytical insight. The most productive developments in the field have consistently emerged from a tight coupling

between physical reasoning and computational capability, with each informing and constraining the other. Machine learning models that violate known conservation laws or produce unphysical symmetry breaking remain a concern, and the incorporation of physical constraints, symmetries, and conservation laws into model architectures through equivariance, gauge invariance, and Noether's theorem remains an active and productive research direction. The physicist's role is evolving from calculator to architect, designing the frameworks within which intelligent computational tools operate and interpreting results in the light of physical understanding.

X. CONCLUSION

Computational physics has passed through several transformative transitions, each opening qualitatively new scientific territory. The formulation of DFT and its proliferating extensions enabled the quantum mechanical treatment of real materials at practical computational cost. The development of classical and reactive force fields extended accessible system sizes by several orders of magnitude. The advent of machine learning interatomic potentials began bridging the accuracy gap between force fields and DFT while approaching the scale of classical simulations. Physics-informed neural networks and equation-discovery methods have introduced AI as a solver and discoverer of physical laws rather than merely a fitting tool. Generative models and large-scale databases are beginning to invert the traditional workflow of materials science, proposing candidates before synthesis rather than rationalizing experiments after the fact.

The field is in a period of rapid and occasionally disorienting change, but the fundamental goals remain unchanged: to understand how matter behaves and to design materials with properties that serve human needs. Computational physics, augmented by artificial intelligence, is better equipped to pursue those goals than at any previous moment in the history of the discipline. The works reviewed here represent the foundations upon which the next generation of breakthroughs will be constructed, and the pace of innovation suggests that those breakthroughs may arrive sooner than even optimistic forecasts have anticipated.

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