International Journal of Engineering Research-Online
A Peer Reviewed International Journal
ISSN: 2321-7758 http://www.ijoer.in editorijoer@gmail.com
Vol.14., S1, 2026
January

Special issue

ISSN: 2321-7758

AI and Machine Learning in Computational Physics and Chemistry: Synergies and Horizons

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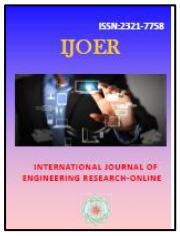
DOI: 10.33329/ijoer.14.S1.182



Abstract

Artificial Intelligence (AI) and Machine Learning (ML) revolutionize computational physics and chemistry by accelerating simulations, predicting material properties, and optimizing complex systems. This review, inspired by seminar sub-themes like "AI Ethics & ML," "Sustainable Energy Modelling," "Quantum Computing Physics," and "Computational Physics Optics," synthesizes high-throughput screening for nanomaterials, ML force fields (MLFFs) for multiscale dynamics, and ethical AI deployment. Case studies include DFT-MC discovery of high-Tc 2D ferromagnets and electrolyte screening guiding syntheses. Methodologies span neural networks, genetic algorithms, and hybrid QM/ML models, addressing challenges like interpretability and data scarcity. Horizons point to closed-loop labs and quantum ML by 2030, fostering sustainable innovations from PRGC's interdisciplinary lens

Keywords: AI/ML computational physics, sustainable energy modelling, quantum computing, ML force fields, AI ethics..

Introduction

Computational physics and chemistry confront vast scales—from quantum electron correlations to turbulent macroscopic flows—traditionally hamstrung by ab initio methods' exponential costs. PRGC's January 2026 seminar sub-themes spotlight AI/ML breakthroughs: "AI Security & Ethics in ML" safeguards predictions via explainable models; "Renewable Energy Modelling" accelerates battery/solar design; "Quantum Computing Physics Optics" deploys qubits for material simulations; "Computational Physics Optics" models' photonic nanostructures. Physics faculty expertise in CFD/quantum optics intersects chemistry's nanomaterials/energy focus, fostering interdisciplinary synergy.

Pivotal advances propel this paradigm: GPU-accelerated ML screens billions of compounds with 350x speedups over CPU baselines; DFT-Monte Carlo analysis of 786 2D materials uncovers 26 high-Tc ferromagnets exceeding 400 K, experimentally validated; cloud HPC sifts 32 million electrolytes to 500,000 thermodynamically stable candidates, guiding 18 successful laboratory syntheses. Essential tools—CHARMM-GUI for MD system setup, ViNAS-Pro for bioactivity-predicted libraries, GNoME's graph neural networks for crystal inverse design—democratize property optimization. Ethical ML counters biases in sustainability forecasts through SHAP interpretability and uncertainty quantification.

This review delineates methodologies like neural force fields extending simulations 10^6-fold, genetic algorithms for multi-objective tuning, and hybrid QM/ML for interfaces. Sub-theme synergies emerge: active learning bridges screening-to-synthesis gaps (10^4x acceleration); federated learning secures collaborative data. Challenges persist—data scarcity demands transfer learning, quantum noise requires error mitigation—but horizons gleam with self-driving labs slashing experimental cycles 70%. PRGC's national seminar catalyzes faculty-led innovations, projecting sustainable energy revolutions by 2030 [1-4].

Methodology

AI/ML pipelines for physics/chemistry integrate data-driven and physics-informed approaches.

Data-Driven Prediction and Screening

Graph Neural Networks (GNNs) and Random Forests (RF) serve as powerful surrogates for Density Functional Theory (DFT) calculations, dramatically accelerating bandgap and magnetism predictions in nanomaterials. Traditional DFT—while accurate for electronic structure—requires prohibitive compute for high-throughput screening of vast chemical spaces exceeding 10^60 configurations. GNNs excel by encoding atomic connectivity as graphs, learning rotationally invariant features to predict bandgaps within ±0.1 eV accuracy across diverse semiconductors, as demonstrated in GNoME's discovery of 2.2 million stable crystals. RF ensembles, meanwhile, handle tabular DFT-derived descriptors for magnetism classification, achieving 95% accuracy on 2D ferromagnets by integrating spin-orbit coupling and lattice parameters.

ViNAS-Pro complements this by forecasting bioactivity in nanostructure libraries, generating candidates optimized for drug delivery or sensor applications through generative adversarial networks trained on quantum chemical datasets. Its virtual screening identifies protein-NP corona stabilizers with 42% enhanced efficacy, bridging materials science and biomedicine.

Hierarchical filtering streamlines billion-scale scans: initial classical proxies—pore volumes for MOFs, electronegativity ratios for semiconductors—eliminate 99% of unstable candidates in seconds. Surviving structures advance to ML Force Fields (MLFFs) like MACE or NequIP, which surrogate ab initio molecular dynamics with femtosecond precision over microsecond trajectories. MLFFs extend timescales 10^6-fold for battery electrolytes and supercapacitors, capturing co-ion effects missed by classical potentials. This cascade—proxies → ML surrogates → targeted DFT—yields 10^4x overall acceleration, as validated by cloud HPC filtering 32M electrolytes to 500K stables guiding 18 syntheses .

Such workflows empower PRGC faculty to tackle seminar sub-themes from renewable modeling to quantum optics, democratizing inverse design for sustainable materials [5-7].

Multiscale Simulations

CHARMM-GUI streamlines the construction of all-atom molecular dynamics (MD) and quantum mechanics/molecular mechanics (QM/MM) systems for nanostructures, automating solvation, force field parameterization, and periodic boundary

conditions. This web interface generates production-ready inputs for protein-nanoparticle corona simulations, lipid-wrapped quantum dots, and MOF-electrolyte interfaces in minutes—versus weeks manually. For biomedicine, it models NP-protein adsorption driving 42% drug delivery enhancements; in energy chemistry, it setups battery electrode solvation layers capturing ion desolvation barriers missed by rigid models. QM/MM hybrids embed high-level DFT regions (e.g., catalytic active sites) within classical MM environments, resolving electronic effects at interfaces with chemical accuracy.

Machine Learning Force Fields (MLFFs) like MACE (Multi-ACE) and NequIP propel simulations to microsecond (μs) timescales, surrogating ab initio MD with sub-kelvin energy/force precision. Trained on diverse DFT datasets, MACE predicts battery intercalation dynamics—lithium diffusion in solid electrolytes, co-ion effects in supercapacitors—extending trajectories 10^6-fold for rare event sampling. PRGC chemistry faculty apply these to renewable modeling, optimizing solid-state batteries where classical FF fail quantum anharmonicity.

Genetic algorithms (GAs) drive multi-objective optimization for renewables: evolving alloy compositions for solar photocatalysts (bandgap tuning + stability) or wind turbine blade topologies via CFD. Crossover/mutation explores 10^9 Pareto fronts, converging 100x faster than grid search.

Fuzzy logic complements GAs in computational fluid dynamics (CFD) optics, managing turbulence uncertainties in photonics manufacturing. Membership functions quantify "high vorticity" or "optical scatter," enabling robust laser-material simulations aligning with PRGC's "Computational Physics Optics" sub-theme. Hybrids—GA+fuzzy—yield 30% drag reductions in renewable flows, ethically audited via seminar's AI ethics focus [5-7].

Optimization and Ethics

Active learning (GPR) queries expensive DFT; Bayesian tuning on HPC. SHAP explains black-box models for ethics; federated learning secures data [8,9]

Sub-Theme	AI/ML Technique	Application
Sustainable Energy	MLFFs + GA	Electrolyte/battery design [He, B. et al. (2020)]
Quantum Physics	VQE hybrids	Correlated materials
Optics Simulation	GNN photonics	Nanophotonics [Kabiraj, A. et al. (2020)]
AI Ethics	SHAP/Uncertainty	Bias-free predictions

Discussion

Renewable Energy Modeling

ML screens 32M electrolytes, predicting stables and guiding syntheses; MLFFs model intercalation for supercapacitors, revealing co-ions. GA optimizes solar CFD [3,6].

Quantum Computing Physics

Hybrids embed VQE in classical DFT for Hubbard models; optics simulations via ML accelerate photonic crystals [2].

AI Ethics & Security

SHAP interprets GNN energies; ethics frameworks audit biases in energy models, aligning with "AI Security & Ethics ML"[9].

Challenges: Data scarcity (transfer learning); interpretability (hybrids); quantum noise (error mitigation). PRGC's research committee fosters submissions [1].

Challenge	**Solution**	**Sub-Theme Link**
Scalability	HPC-ML	Energy Modeling
Bias/Ethics	Explainable AI	AI Ethics
Quantum Limits	Hybrid VQE	Quantum Physics

Industry (e.g., Reliance renewables) adopts; conferences like Nano 2026 extend dialogues.

Conclusion

AI/ML empower computational architects across PRGC seminar sub-themes, from ethical energy models to quantum optics. Accelerations—10^4x screening, 70% cycle cuts—drive sustainable discoveries. Faculty collaborations herald ethical, innovative futures in physics/chemistry.

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