THE ROLE OF ARTIFICIAL INTELLIGENCE IN COMPUTATIONAL MATERIALS SCIENCE AND CONDENSED MATTER PHYSICS

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Abstract:
Artificial Intelligence (AI) has emerged as a transformative force in computational materials science (CMS) and condensed matter physics, leveraging its integration with Density Functional Theory (DFT)- a robust tool for atomic-scale understanding- to precisely analyze and predict complex material behaviours, thereby accelerating discovery. In this study, we examine the state of AI in computational materials science today, with a particular emphasis on DFT. We go over how AI is being used in DFT, such as creating new exchange-correlation functionals, predicting material attributes, and optimizing DFT computations. This study examines how DFT procedures are being revolutionized by machine learning (ML) and deep learning (DL) techniques, from predicting new materials with customized properties to accelerating electronic structure computations. We discuss key applications of AI in high-throughput screening, phase transition prediction, and defect modelling, while addressing challenges such as data scarcity, model interpretability, and computational costs.
Keywords: Density Functional Theory, Machine Learning, Computational Materials Science, Condensed Matter Physics, DFT acceleration, Kohn-Sham potential.

1. Introduction:

Artificial intelligence (AI) is a field that is dedicated to researching and developing theoretical frameworks and application systems for simulating and enhancing human brain ability. The primary goal of AI is to enable machines to simulate and replicate intelligent human behaviours such as learning, reasoning, thinking, and planning. The merging of physical sciences and deep learning offers promising opportunities for theoretical research, offering profound insights into the learning mechanisms and computational capabilities of deep neural networks.

Although the field of artificial intelligence (AI) research was founded in the 1950s, its technical applications have gained popularity and public recognition in the last ten years. With the introduction of deep learning in 2012 and the transformer architecture in 2017, the discipline saw significant advancements. In the last five years, the use of AI techniques for scientific research, or AI for science, has gained prominence, especially following the discovery of protein folding. However, physicists were already utilizing AI techniques in particle physics as early as the 1990s. Before 2010, the first machine learning applications to molecular dynamics simulations appeared, and conventional machine learning techniques sped up important discoveries like the 2012 discovery of the Higgs boson.

Computational materials science is a rapidly growing field that aims to understand the behaviour of materials at the atomic scale. DFT is a widely used method for studying the electronic structure of materials and has been instrumental in predicting the properties of a wide range of materials. However, DFT calculations can be computationally intensive, and the development of new materials with specific properties requires a deep understanding of the underlying physics [1]. The integration of computational materials science and artificial intelligence (AI) has created new opportunities for understanding and developing functional materials. The use of AI in computational materials science has attracted a lot of interest recently. Large dataset analysis, predicting material properties, and DFT calculation optimisation have all been accomplished with AI. For instance, novel exchange-correlation functionals for DFT have been created using machine learning methods, increasing the precision of DFT computations [2]. AI has also been used to forecast material characteristics like conductivity and bandgap [3].

AI has long been used in computational materials research. Researchers started looking into using machine learning methods to forecast material qualities in the early 2000s [4]. But AI didn't start to take off in the industry until deep learning algorithms were developed. The promise of AI in computational materials science has been shown in recent works. For instance, scientists have employed machine learning techniques to forecast material characteristics like conductivity and bandgap [5]. Additionally, DFT calculations have been optimized using AI, which lowers the computing cost and increases the correctness of the results [6]. A recent work by [7] showed how well AI predicts material properties using DFT.

2. Applications of AI in DFT

AI has been applied in various ways in DFT, including:

2.1 Development of novel exchange-correlation functionals: AI has been utilized to develop new DFT exchange-correlation functionals, which have increased the precision of DFT computations [8]. For instance, scientists are developing novel functionals that can precisely predict material properties using machine learning techniques [9].

2.2 Prediction of material properties: Artificial intelligence (AI) has been used to forecast material properties, including conductivity and bandgap [10]. For instance, researchers have employed machine learning algorithms to forecast a material's bandgap, a crucial characteristic for figuring out its electronic behaviour [11].

2.3 Optimization of DFT computations: AI has been applied to optimize DFT computations, lowering the computational expense and increasing the precision of the outcomes [12]. For instance, researchers have optimized the basis set and exchange-correlation functional, two parameters utilized in DFT computations, using machine learning techniques [13].

2.4 Reduction of computational costs: Neural network potentials (e.g., SchNet, DeepMD) approximate electron densities and energies, bypassing iterative Kohn-Sham equations [14]. Transfer learning leverages pre-trained models to predict properties of new materials with minimal data [15].

We provide a number of case stories to demonstrate AI's potential in DFT. For instance, scientists have employed machine learning algorithms to forecast material characteristics like conductivity and bandgap. Additionally, AI has been applied to optimize DFT computations, lowering computing costs and increasing result accuracy.

3. AI-Powered DFT Tools

To help researchers in DFT calculations, a number of AI tools are being created. Here are a few instances:

3.1 DFT+ML: A machine learning framework for DFT-based material property prediction [16].

3.2 Materials Genome Initiative: This project uses DFT and AI to create a comprehensive database of material properties [17]

3.3 Deep learning-based DFT: A deep learning-based method for DFT-based material property prediction [18].

4. Condensed Matter Physics with AI

4.1 Phase Diagram Mapping: In spin systems, hidden order parameters can be found using unsupervised learning techniques such as autoencoders. Analytical formulations for phase boundaries are found by symbolic regression [19].

4.2 Quantum Materials Design AI helps find:

4.2.1 Topological materials:

GNNs (Graph Neural Network) use band structures to categorize Chern numbers [20].

4.2.2 Superconductors:

Critical temperature (Tc) is predicted from atomic properties using Bayesian optimization [21].

4.3 Engineering Defects:

Stable defect configurations are suggested by generative models [22]. Defect-property connections are revealed by explainable AI (e.g., SHAP analysis) [15].

5. Challenges and Future Directions

Even though the use of AI in DFT has advanced significantly, there are still a number of challenges and restrictions that must be overcome. These include the interpretability of AI models, the complexity of material behaviour, and the requirement for big datasets. The creation of more precise exchange-correlation functionals, the use of AI in complicated materials systems, and the combination of AI with other computing techniques are some of the future directions for AI in DFT**.**

6. Conclusion

In conclusion, artificial intelligence (AI) has become a potent tool in computational materials science, allowing researchers to examine the behaviour of complicated materials and make previously unheard-of predictions about their properties. The application of AI in DFT has shown tremendous potential, and we hope to see ongoing breakthroughs in the sector. We believe that AI will become more crucial in the search for novel materials with certain characteristics as the area develops.

7. Future Work

Future research in this field will concentrate on creating exchange-correlation functionals that are more precise, applying AI to intricate material systems, and combining AI with other computing techniques. Additionally, we believe that AI will be crucial in the development of novel materials with particular characteristics, like enhanced energy storage materials and high-temperature superconductors.

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