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REGULAR ARTICLE

Leveraging Artificial Intelligence to Predict Electronic Structures in Nanoparticles

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The application of artificial intelligence (AI) techniques in predicting electronic structures of nanoparticles is a complex task traditionally reliant on quantum mechanical calculations. The unique properties of nanoparticles, driven by quantum confinement effects at the nanoscale, are crucial in fields such as catalysis, electronics, and medicine. The study utilize advanced computational models, specifically Adaptive Tunicate Swarm Optimized Graph Neural Networks (ATSO-GNN), to accurately predict electronic density, energy states, and other properties of nanoparticles. The approach comprises data preprocessing with *z*-score normalization and feature extraction utilizing Linear Discriminant Analysis (LDA), which improves model sensitivity to minor electrical fluctuations. The ATSO-GNN model, trained on structural data from a nanoparticle dataset, demonstrates significant improvements in accuracy and computational efficiency over traditional methods like Density Functional Theory (DFT). Results indicate that the approach effectively captures complex atomic interactions, making it valuable for materials science and nanotechnology applications where rapid and precise electronic structure predictions are essential. Compared to standard methods, the ATSO-GNN model offers higher R^2 (0.95) lower mean absolute error (MAE) (0.2) and lower computation times (1.5) enhanced prediction. This study demonstrates how AI-based methods significantly improve the speed and accuracy of electronic structure predictions.

Keywords: Nanoparticles, Electronic structure prediction, Machine learning, Density functional theory, Nanotechnology.

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1. INTRODUCTION

Electronic structures are the arrangement and behavior of electrons in atoms, molecules, or materials and become important in determining the chemistry and physics of nanoparticle properties [1]. The effects due to quantum confinement, relevant to the size reaching nanoscale, make its electronic structures highly different compared with bulk materials. Such effects lead to discrete energy levels rather than continuous bands, thereby influencing the optical, electrical, and magnetic properties of nanoparticles [2]. Such unique properties make nanoparticles essential in various applications, including catalysis, where they enhance reaction rates; electronics, where they enable faster and more efficient devices, and medicine, where they aid in targeted drug delivery and imaging. Understanding and controlling the electronic structures of nanoparticles thus leads to the development of advanced materials with tailored properties suited for specific applications [3]. Prediction of electronic structures is a highly challenging problem and largely stems from the quantum mechanical computation involved. This would require a solution to many interacting electrons in solving Schrodinger's equation with increasing system size [4]. The difficulty related to electron-electron correlations and high levels of accuracy required to determine the wave functions and their density are the difficulties related to increasing complexity [5]. There are only approximations, and usually fail in systems with important electron correlations or excited states. With advanced computational methods, large molecules or materials, and much computing time, electronic structure predictions can be made very accurate; this remains an exciting but

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difficult challenge area in materials science and quantum chemistry [6]. AI significantly improves and simplifies the electronic structure prediction through using more complex algorithms that can analyze large datasets and optimize computations. Deep learning (DL) and neural network (NN) are among the best ML models in pattern recognition in large data sets, which facilitates better and more efficient prediction of electronic structures [7]. This accelerates traditionally resource-intensive methods, such as density functional theory (DFT), by predicting properties, such as electronic density and energy states with similar precision but at a significantly lower computational cost [8]. AI models also have the ability to generalize from vast libraries of known structures, making them proficient at predicting properties for new or complex materials where experimental data can be scarce [9]. This efficiency supports the fast discovery in fields, such as material science and quantum computing allows faster innovation with fewer time and resources [10]. The purpose of this study is to develop and apply AI techniques for predicting an accurate electronic structure of nanoparticles. The task is accomplished with the help of AI algorithms by streamlining traditionally very complex, computationally intensive processes traditionally required for electronic structure calculations.

2. RELATED WORKS

An early technique for identifying the form of nanoparticles' metal cores four alternative supervised artificial neural network (ANNs) [11] were trained, evaluated, and applied to a difficult dataset. The use two structural descriptors: Radial Distribution Functions (RDF) and Coulomb Matrices (CM). Nano architectonics is a new type of nanomaterial with self-assembled atoms and distinctive characteristics. Nano architectonics has potential uses in catalysis, solar energy storage, water and wastewater treatment, sensing, fuel cells, medicines, and medication delivery, among other fields [12]. An ANN [13] is a wide approach for forecasting a rather generic characteristic, and in a few configurations presented, the total energy of any gold nanoparticles is rectified using an embedded atom potential and the self-consistent charge density functional bounding method. As AI technology progresses, it plays a growing role in material science and engineering (MSE) [14]. High-performance computing allows for testing deep learning (DL) models with large parameters, overcoming the limitations of previous approaches like DFT in property prediction. Nanoparticles have unique features that make them indispensable in optoelectronic sensing, medicinal treatment, material science, and chemical applications. Nanoparticles can be created using many synthetic methods, each with unique features [15]. AI technology can handle complex tasks with human-like skill. AI breakthroughs have a significant impact on ML, which is used to solve a variety of challenges, including nanotechnology.

3. METHODS AND MATERIALS

The method includes data preprocessing with z-score normalization and feature extraction using LDA, which increases model sensitivity to tiny electrical oscillations. The ATSO-GNN model was trained on structural data from Kaggle's nanoparticles dataset.

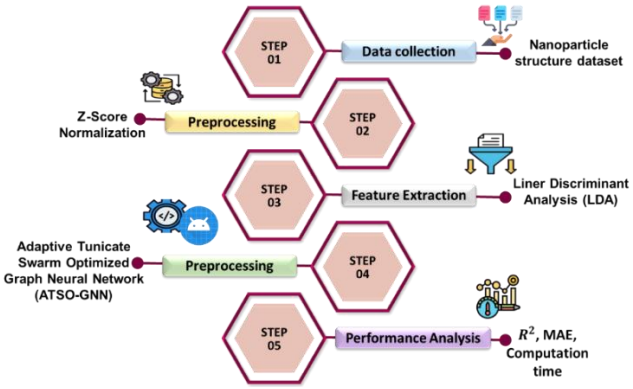

Fig. 1 – Flow of proposed

3.1 Data Collection

The dataset was collected from an open source Kaggle website((https://www.kaggle.com/datasets/ziya07/nanoparticle-electronic-structure/data) dataset features structural and atomic properties of nanoparticles, including atom count (19-140 atoms), structure type (cuboctahedral, icosahedral, or cubic), atomic number (noble metals like Pt or Au), electronegativity (2.0-3.0), atomic radius (in Å), and melting point (in Kelvin). Additionally, it includes 50 principal components (dos_pc1 to dos_pc50) from PCA-transformed synthetic density of states (DOS) data, condensed from 3000 levels to capture key electronic variations.

3.2 Data Preprocessing Using *z*-score Normalization

In the electronic structures of nanoparticles, z-score normalization is a common data preprocessing technique applied to standardize the dataset by centering the values on zero with unit variance. This process helps in enhancing the model's sensitivity to subtle variations in electronic properties by removing scale biases and facilitating more accurate analysis of nanoscale behavior. This is very crucial for proper comparison and analysis of data, especially in electronic structures in nanoparticles studies where standardization is crucial in carrying out an accurate examination of electronic behavior across varied sample conditions in equation (1).

$$P = Y - \frac{\mu}{\sigma} \tag{1}$$

This paper will enhance logistics distribution through the use of a statistical method that employs standard deviation and mean to measure performance indices, thus contributing to better insight into the effect of electronic

structures on the efficiency and effectiveness of nanoparticles logistics in equation (2).

$$\sigma = \sqrt{(\sum (Y - \bar{Y})/o)} \quad (2)$$

To analyze the comprehensive dataset, including standard deviation, mean, and frequency, to assess the impact of electronic structures in nanoparticles on the global market for products and services. This analysis aims to derive insights into supplier performance and product distribution trends, contributing to a deeper understanding of logistics efficiency and its correlation with electronic properties in nanomaterials. This objective aligns the data analysis aspect with the broader context of electronic structures in nanoparticles, potentially exploring how these materials influence market dynamics.

3.3 Feature Extraction Using Linear Discriminant Analysis (LDA)

Exploring electronic structures in the nanoparticles permits the feature extraction of unique quantum and physical properties of nanoscale material. LDA applied to these structures permits the small dissimilarities between the nanoscale particles to be identified. It increases the efficiency of classification in materials analysis. The electronic feature separation is maximized by LDA. Given a set of independent data attributes, LDA generates a linear combination that optimizes the average variation between the intended classes. Two key measures are defined in LDA, with one being the within-class scatter matrix, given by equation (3).

$$Sw = \sum_{i=1}^{d} \sum_{j=1}^{M_i} (w_j^i - \mu_i)(w_j^i - \mu_i)^S \quad (3)$$

Where w_j^i is the i^{th}sample of class j, μ_i is the denote of class$j$,d is the numeral of classes, and μ_i is the numeral of sample in class j. Additionally, the among-class distribute matrix can be calculated using equation (4). Where μrepresent the denote of all classes.

$$Sb = \sum_{i=1}^{d} (\mu_i - \mu)(\mu_i - \mu)^S \quad (4)$$

3.4 Predicting Electronic Structures in Nanoparticles Using Adaptive Tunicate Swarm Optimized Graph Neural Network (ATSO-GNN)

In these nanoparticles, the electronic structures play a crucial role in enhancing the capabilities of adaptive algorithms. These features, in this Adaptive Tunicate Swarm Optimized Graph Neural Network (ATSO-GNN), enhance the ability of the model to catch intricate interactions and patterns at the nanoscale level. This approach holds huge promise towards the development of nanotechnology applications, particularly in material and biomedical fields.

3.4.1. Graph Neural Network (GNN)

GNN is very useful for the study of electronic structures in nanoparticles because it captures complicated relationships between atoms efficiently. Letting the nanoparticle structure be graph-based, where nodes are atoms and edges represent bonds, GNN can predict properties like electronic density, energy states, and distribution of charge. The second step involves a formal aggregate operation. This simple type of GNN has a constant message carrying function, and the aggregation is simply adding all of the information that the neighbor passes onto it for summarization. It is not difficult to see that can improve GNN performance in at least three ways: picking strategy, aggregating function, and stacking layers. For example, if the relevance of neighbors to the center node varies, they can apply the attention mechanism at the first step of the aggregate function can offer a general formulation of GNN equation (5).

$$g_{out}^{(l)} = Update\left(Aggregate\left(g_v^{(l-1)}, \forall v \in M(v)\right\}, X_{agg}^{(l)}\right), g_{in}^{(l)}, X_{Update}^{(l)}) \quad (5)$$

The terms $g_{in}^{(l)}$ and $g_{out}^{(l)}$ refer to the effort and modernized node embedding at the l^{th}coating, respectively. The embeddings of neighbors from the preceding layer are represented by $g_v^{(l-1)}$ and u. $X_{agg}^{(l)}$ and $X_{Update}^{(l)}$represent trainable matrix in collective and inform functions at the l^{th} layer, respectively. $X_{Update}^{(l)}$ update refers to the trainable parameters of the l^{th} layer in neural networks following the collective function. Figure 2 depicts the overall structure of GNN.

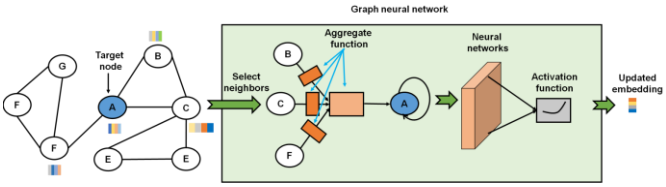

Fig. 2 – Structure of GNN

Electronic Structures in Nanoparticles: A generic and simple GNN structure and processing mechanism. First, GNN chooses neighbors using a predetermined strategy. Then, GNN uses an aggregated function to retrieve information about a central node. Finally, the aggregated data is passed to a neural network, which performs the nonlinear transformation. The final result is the modified central node description in equation (6).

$$g_v^{(l)} = \sigma([B_l.AGG\left(\left\{g_v^{(l-1)} \forall v \in M(v)\right\}\right), A_l g_v^{(l-1)} \quad (6)$$

Where $g_v^{(l)}$ and $g_v^{(l-1)}$represents node v at presentcoating$l$ and preceding coating$(l-1)$, respectively. Furthermore, $g_v^{(l-1)}$ represents the node embeddings of nodes of the neighbors from the preceding layer. $A_l$and B_l represent the trainable weight matrices. σrepresents a quadratic function of activation. To create$g_v^{(l-1)}\forall$, follow these procedures. To begin, each node uses the aggregator to aggregate features from its immediate neighborhood

into a single vector, $M(v)$. After aggregating neighbor features, Graph concatenates the node's prior representation with its neighborhood feature vector. The concatenated vector is sent through a multi-layer perceptron (MLP) with rectified linear unit (ReLU) activation function, resulting in a new representation of the node. A graph learning job is an optimization problem, similar to supervised learning where input w is supplied and label z is predicted in equation (7).

$$\min_{\Theta} K(z, e(w)) \tag{7}$$

To optimize a set of parameters Θ and use a loss function (L). The GNN function (f) can be quite complicated. F generates node predictions as its output. The objective is to minimize the loss between predicted and real labels.

3.4.2 Adaptive Tunicate Swarm Optimization (ATSO)

The electronic structures in nanoparticles with ATSO is introduced via a new searching equation, which improves the exploitation ability for resolving large-scale problems and aversion to trap into a local optimum. The key steps of the ATSO are as follows.In the context of electronic structures in nanoparticles, the algorithm begins with

Step 1: The algorithm parameters, such as the increasing number of generations T and inhabitant'sdimension, are set. ATSO then randomly positioned within the investigate space.

Step 2: Then, every tunicate is evaluated using the fitness function.

Step 3: In the development phase, the focus is on enhancing the ATSO's search process. A dynamic perturbation is introduced to sharpen the exploitation pattern and to explore nearby solutions with the search area. The search equation is modified so that each position experiences a dynamic step change, retaining its place if it produces an improved result. This method allows for continuous updating of the search space boundaries, with the new ATSO position specified in equation (8).

$$O_{pop}(s=1) = O_{pop}(s) \pm rand^{s} \times \frac{\alpha}{2} \tag{8}$$

For electronic structures in nanoparticles, the optimization process involves a dynamic step reduction to enhance the focus on neighborhood searching, thereby improving exploitation capabilities. This can be represented in equation (9):

$$\alpha = \theta \times \alpha_1 + (1-\theta) \times \alpha_2 \tag{9}$$

The study of electronic structures in nanoparticles, $\bar{O}_{pop}$ represents a random variable (RV) following a uniform distribution between 0 and 1, withα_1 and α_2 defining the dynamic bounds, calculated as shown in equation (10).

$$\alpha_1 = \min(\bar{O}_{pop}), \alpha_2 = \max(\bar{O}_{pop}) \tag{10}$$

Step 4: Updating phase: In this phase, the tunicate swarm is refined to the standard ATSO method using equation (10). This process enables the tunicates to explore different areas with the search space, boosting their exploratory potential. Subsequently, the fitness of each tunicate is evaluated to determine and update the current optimal solution.

Step 5: Steps two to four could be repeated if the termination criterion is met. Equation (9) enhances exploration by allowing examination of additional areas with the search region, especially in the study of electronic structures in nanoparticles. Equation (10), is valuable for concentrating on promising regions, thus supporting exploitation. This approach establishes a balance between exploration and exploitation, helping to prevent entrapment in local optima.

4. RESULT AND DISCUSSION

Utilizing AI in predicting electronic structures in nanoparticles improves the efficiency and accuracy of computations in the rapid discovery and optimization of new materials. The approach used the electronic properties of materials in fields like nanotechnology, electronics, and catalysis. An Intel 16 GB of DDR4 RAM, Xeon E3-1230v5 CPU, and an NVIDIA Quadro K420 discrete graphics card power the system. It also has a 1TB SSD, guaranteeing express and successful storage. Comparison of our proposed method with the standard approaches, such as metrics of R^2, MAE, and computation time.

4.1 *R*-Square

In the context of predicting electronic structures in nanoparticles using statistical modeling, an R-squared (R^2) value indicates the amount of the variation in the dependent variable can be explained by its separate factors. A good proportion of the variance in the electronic

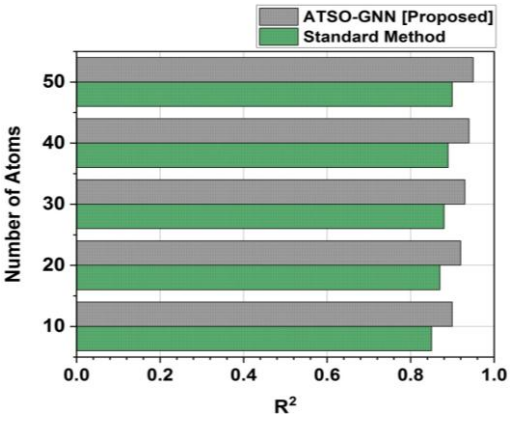

Fig. 3 – Analysis of R^2

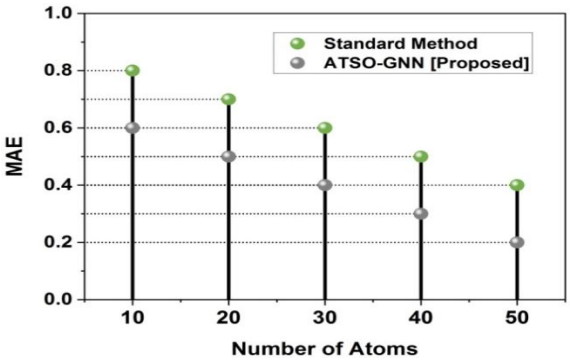

Fig. 4 – Analysis of MAE

structures can be accounted for the model if the R^2 value is close to 1, thus, a good fit. On the contrary, if the R^2 value approaches 0, then it means that the model cannot explain the variation and the modeling techniques require improvement or more relevant features are required to be added. Fig. 3 displays the result of R^2.

4.2 MAE

The Mean Absolute Error (MAE), a statistical metric that evaluates the accuracy of forecasts or predictions is the average absolute difference between the expected and actual values. Analyzing these electronic structures will lead to designing nanomaterials that would be applied in catalysis, energy storage, or electronic devices and such materials could enhance the engineering applications. Fig. 4 represents the results of MAE.

5. CONCLUSION

The traditional quantum mechanical methods, although accurate, are computationally intensive and restricted by the complexity of electron-electron interactions. ATSO techniques incorporated in GNN models help model atomic and molecular interactions at the nanoscale with precision. Techniques such as adaptive tunicate swarm optimization help optimize performance metrics with much higher precision. AI-driven innovation has enabled faster, resource-efficient innovation in material science and quantum computing and continues to advance nanoparticle material development with high precision and applicability. When compared to standard methods, the proposed higher R^2(0.95), lower MAE (0.2), lower computation time (1.5) method ATSO-GNN had effectively.

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Використання штучного інтелекту для прогнозування електронних структур у наночастинках

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Застосування методів штучного інтелекту для прогнозування електронних структур наночастинок є складним завданням, яке традиційно залежить від квантово-механічних розрахунків. Унікальні властивості наночастинок, зумовлені ефектами квантового обмеження на нанорівні, мають вирішальне значення в таких галузях, як каталіз, електроніка та медицина. У дослідженні використовуються передові обчислювальні моделі, зокрема адаптивні нейронні мережі з оптимізованим графічним методом адаптивного рою тунікатів (ATSO-GNN), для точного прогнозування електронної густини, енергетичних станів та інших властивостей наночастинок. Підхід включає попередню обробку даних з нормалізацією *z*-оцінки та вилучення ознак з використанням лінійного дискримінантного аналізу (LDA), який покращує чутливість моделі до незначних електричних коливань. Модель ATSO-GNN, навчена на структурних даних з набору даних про наночастинки, демонструє значні покращення точності та обчислювальної ефективності порівняно з традиційними методами, такими як теорія функціоналу густини (DFT). Результати показують, що цей підхід ефективно фіксує складні атомні взаємодії, що робить його цінним для застосування в матеріалознавстві та нанотехнологіях, де швидкі та точні прогнози електронної структури є важливими. Порівняно зі стандартними методами, модель ATSO-GNN пропонує вищий R2 (0,95), нижчу середню абсолютну похибку (MAE) (0,2) та коротший час обчислення (1,5), що покращує прогнозування. Це дослідження демонструє, як методи на основі штучного інтелекту значно покращують швидкість і точність прогнозування електронної структури.

Ключові слова: Наночастинки, Прогнозування електронної структури, Машинне навчання, Теорія функціоналу густини, Нанотехнології.