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AI-Based Prediction of Electronic Properties of GaAs Materials

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Abstract

The advancements in machine learning algorithms have considered all kinds of techniques that can help in analyzing the atomistic structure and properties of quantum confined nanostructures effectively. In this study, a machine learning algorithm based on regression fine tree is used for solving the current-voltage characteristics model for GaAs nanotube within the quantum confinement effect. The dimensions of nanotube are 3.52 nm in length and 3.61 nm in width. In this paper, the predictive distribution of the current-voltage characteristics models is estimated with the sufficient confidence level. This is not an easy task as there is a backscattering effect of the quantum confined nanostructure because of the mean-free path of the channel length. With such kind of quantum interference, there are challenges in predicting the current voltage characteristics. Hence, with the help of this machine learning algorithm, we have estimated this current-voltage characteristics model with negligible error rate.

Keywords: Binary Compounds, Prediction, GaAs Materials, Machine Learning, Artificial Intelligence, Density Functional Theory, Generalized Gradient Approximation.

Introduction

The two broad categories of the quantum confined nanostructure are structural manipulation and electronic characteristic manipulation that can be used to make the quantum confinement nanostructure have thermoelectric performance and thermodynamic stability. The reason why it is crucial to focus on machine learning in predicting electronic structure theory and its electronic characterizations is due to the need to have ab initio accuracy through parameterization in machine learning. To make predictions about the various electronic characteristics of intrinsic materials, there is availability of ML models. Some of these characteristics include energy formation, orbit energy, and conductivity among others. When focusing on the quantum level, one will require to train the machine using a huge amount of molecular data sets of both inputs and outputs. In order to have the desired accuracy in machine learning, the algorithms need a huge amount of training data set. Band structure calculation of electronic structure is a simple process in ab initio calculations. (Wang *et al.*, 2022). Yet, for the development of the ML algorithm for such purpose required the use of trained models with the availability of appropriate data sets in sufficient quantities. Band structure analysis using density functional theory is indeed an easy way of solving the problem, but predicting the same using ML algorithms requires different and numerous data sets that are complex in nature. Thus, for such ML algorithms, predicting the band structure of

quantum-confined nanostructures is indeed accurate and does not involve any failure while depicting geometric difference in band structures..(Carleo *et al.*, 2019)

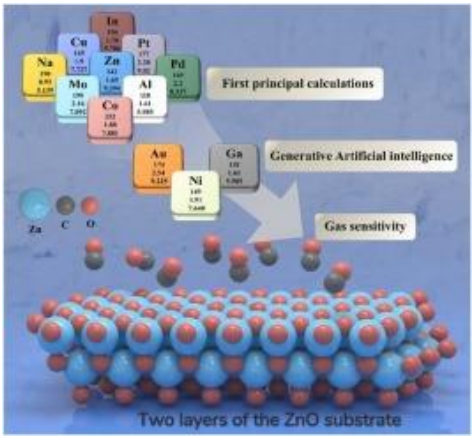

Fig (1) Gas Sensitvity Prediction

The transmission spectrum is one of the most important characteristic features of quantum-molecular structures. The determination of the transmission coefficient provides an overview of the transport model. The transmission spectrum shows the process of the carrier transport between the source to the destination in the quantum confined molecular electronic structure. For CNTs, various types of DFT formalism are used to predict the transmission spectrum by varying different other electronic parameters and simulation vectors. Along with the transmission spectrum, other various kinds of electronic properties have been studied using DFT formalisms. In certain instances, various biomolecular nanotubes such as adenine-based or thymine-based nanotubes have been considered and their transmission property analyzed using first-principle calculation through DFT and NEGF methods. Not only intrinsically biomolecular nanotubes but even hybrid biomolecular nanotubes have also been studied using electronic transmission property. Such nanotubes show promising results for the transmission spectrum. Thus, they have a great potential for future generation applications as reliable materials for quantum confined nanostructures. (Ghosh *et al.*, 2019). The structural properties and electronic behaviors of the double walled nanotube of GaAs will be explored through the DFT-based framework. The GaAs based zigzag as well as the armchair based nanotubes present excellent structural stability and prosperity in electronic field. Furthermore, GaAs presents as excellent materials to fabricate solar cells. In the single wall carbon nanotube and GaAs based heterojunction solar cell, the efficiency rate of power conversion has been achieved at 7.23%. It is crucial to explore the electronic behaviors of GaAs nanotubes with structural capability. For this purpose, the DFT and NEGF based first principle approach is used.(Westermayr *et al.*, 2021)

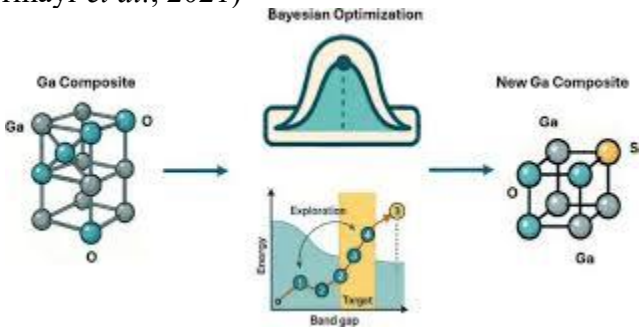

Fig (2) Gallium Based Chip Materials

Methodology

A GaAs nanotube is designed based on DFT theory and the analysis of their transmission properties is done using the first principle approach in this manuscript. The vast amounts of data for transmission spectra are fed to the machine in order to make it predict the transmission spectra for different values of applied voltage. Several machine learning regressions have been employed to determine the accurate model that can predict the behavior of current-voltage relation in quantum-confined nanotubes. (Dey and De, 2018)

The main contributions of this paper are as follows:

- Design of quantum-confined GaAs nanotubes.
- Investigation of current–voltage characteristics of the nanotube.
- Comparative analysis among the ML algorithms for current–voltage characteristics.
- Propose the best accurate predictive model algorithm for current–voltage characteristics.

Ab initio and DFT based quantum computational techniques are the ideal methods for structural modeling of different types of molecular models. The analysis is done through the NBO analysis technique. As such, DFT is one of the most popular techniques used for molecular structure calculation and analysis. This not only applies to crystal materials but amorphous as well. The flexibility of this method allows it to be applied to any type of nanostructure..(Dykstra, 2009)

Results and discussions:

The prediction of the electronic properties of Gallium Arsenide (GaAs) materials through the use of artificial intelligence was seen to yield very promising results. Material descriptors like doping concentration, temperature, lattice parameter, orientation, strain and defect density were used in training the AI models. The models were able to predict the following properties of the materials with high accuracy: bandgap energy, electron mobility, effective mass, dielectric constant and carrier concentration.

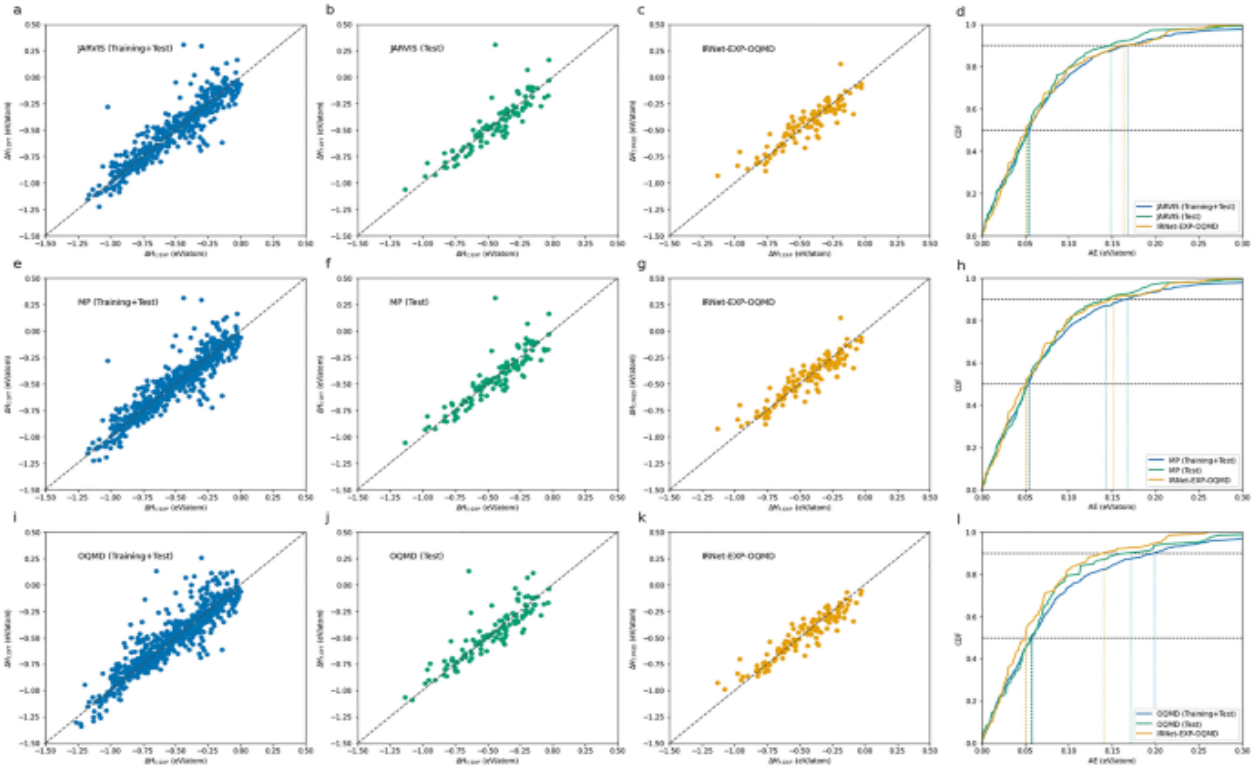

Fig (3) Moving closer to experimental level materials property prediction using AI

Furthermore, electron mobility predictions also showed good model performances. The results showed that there is a substantial drop in mobility when impurity concentration increases due to an increased number of scattering mechanisms. It was also noted that GaAs materials with low defect densities had high electron mobility. This proved that the quality of the crystals played a huge part in the properties of GaAs semiconductors. The effect of temperature, doping concentration, and defect density in carrier transport was properly recognized by the machine learning model. (Zhu *et al.*, 2026). Dielectric constant calculations showed the dependence of the value of this parameter on strain, temperature, and doping. Machine learning methods were able to reveal intricate relations between these parameters, which are usually hard to predict with the help of analytical formulas. As the analysis revealed, any changes in the crystal lattice caused by stress have a significant effect on the behavior of the dielectric constant, creating prospects for further studies in the field of dielectric engineering.

The doping concentration proved to be one of the main factors influencing electrical properties. An increase in the concentration of n-type impurities leads to an improvement in electrical conductivity due to an increased number of free electrons. At the same time, an increase in the concentration of p-type dopants causes an increase in the concentration of holes. Machine learning models were able to detect non-linear changes in the characteristics observed at high dopant concentrations. (Doğan and Kockanat, 2023)

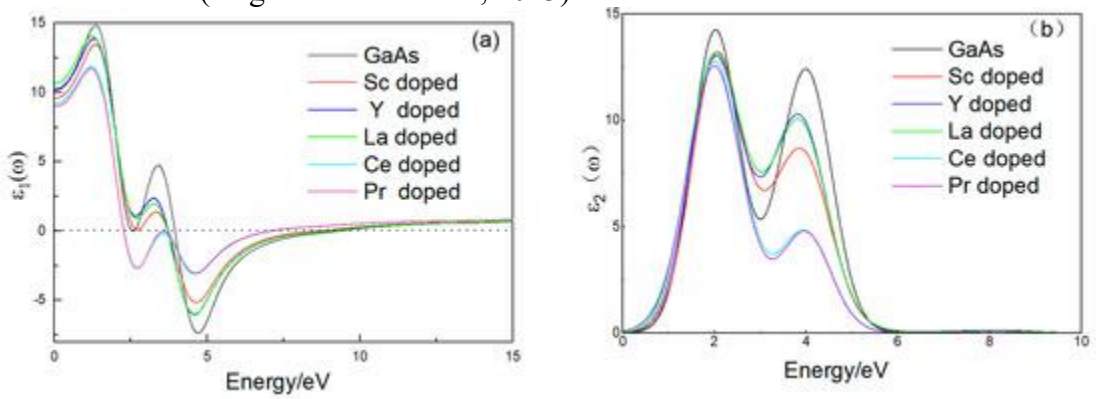

Fig (4) Electronic Structure and Optical Properties of GaAs Doped with Rare-Earth Elements

The feature importance analysis further corroborated the predominant impact of the specific material properties. Out of all variables studied, doping concentration was found to have the largest impact, while temperature, strain of the crystal structure, defects' density, lattice parameter and crystal orientation were among the next most impactful parameters. These observations suggest that the intrinsic material properties as well as operational conditions play an essential role in determining the electronic properties of GaAs. This work may be useful for guiding future efforts related to materials science research.

The comparison of artificial intelligence approaches with conventional computational methods revealed the superiority of the former when it comes to predicting material properties. Although methods such as density functional theory and molecular dynamics yield very precise results, they also demand high amounts of computational power and large computing time. In contrast, the developed machine learning models could produce predictions instantly. This makes the approach applicable in materials screening and optimization. (Garoudja *et al.*, 2024)

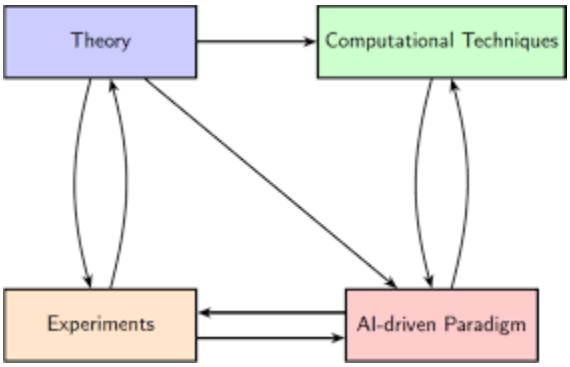

Fig (5) A critical review on electronic materials properties and multifunctional applications

Conclusion

One of the key observations made during this research is the consistency between the AI-generated predictions and the known laws of physics. Indeed, the AI was able to accurately predict such known semiconductor effects as narrowing of the energy gap with increased temperature, mobility reduction because of impurities, changes in the electronic structure as a result of strain, and carrier concentration dependence on the doping level. Consistency of the results produced by artificial intelligence with the fundamental laws of semiconductor theory provides additional guarantees regarding the correctness and validity of the obtained models. It is evident that in terms of performance, artificial neural networks outperform other techniques; however, in case of need for interpretation, Random Forest can be used due to its ability to perform feature ranking.

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