AI-Driven Optimization for Semiconductor Nanodevice Modeling

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***Abstract:** This research aims to enhance quantum mechanical modeling of semiconductor nanodevices by automating basis selection through artificial intelligence (AI). The approach involves developing a comprehensive database of optimized basis representations and training AI models to interact with quantum code libraries, enabling efficient identification and prediction of suitable bases. By reducing computational complexity, minimizing manual intervention, and standardizing simulations across diverse device architectures, this AI-driven automation enhances computational efficiency and scalability. The outcomes of this research have the potential to accelerate semiconductor design and simulation, making advanced modeling techniques more accessible to both academic researchers and industry professionals.*

I. Introduction

The advancement of semiconductor nanodevices relies heavily on accurate modeling at the quantum mechanical and atomistic levels. These models are essential for understanding charge transport, electronic structure, and device performance. However, quantum mechanical simulations are computationally expensive due to the high-dimensional matrices involved in solving Schrödinger and Poisson equations. The complexity of matrix multiplications and inversions scales rapidly with device size, making full-scale simulations infeasible for large systems.

To address this computational challenge, researchers employ low-rank approximations, which significantly reduce the dimensionality of these matrices while maintaining the essential physics of the system. While effective, these approximations require a change of basis, where the original representation of the system is transformed into a lower-dimensional space. The choice of basis is critical and typically optimized for each specific device, often requiring manual intervention and domain expertise. This reliance on device-specific basis functions limits scalability and standardization in semiconductor modeling.

Our research aims to overcome these limitations by developing a comprehensive database of device-specific basis representations and leveraging artificial intelligence (AI) to automate the selection and prediction of basis transformations. The AI model will be trained to utilize quantum code libraries, autonomously selecting the most efficient basis representations for different semiconductor architectures. Eventually, the AI system will be capable of predicting appropriate basis representations without requiring explicit tool intervention, thereby streamlining quantum mechanical simulations.

By integrating AI-driven automation into semiconductor modeling, we aim to enhance computational efficiency, reduce manual optimization efforts, and standardize basis selection methodologies across various semiconductor devices. This research has the potential to accelerate device simulation workflows, making quantum mechanical modeling more accessible and scalable for both academic research and industrial applications.

II. Methodology

Our research involves extensive quantum mechanical simulations of semiconductor nanodevices using Purdue's Nanoelectronics Modeling Tools (NEMO5) software, executed on Negishi, a high-performance supercomputer provided by the Rosen Centre for Advanced Computing (RCAC). The methodology is structured into several key phases:

1. Input Deck Configuration

We begin by defining input decks for a variety of semiconductor materials, including:

- Binary III-V compounds: AlAs, GaAs, InSb, InAs, InP
- Group IV semiconductors: Silicon (Si)

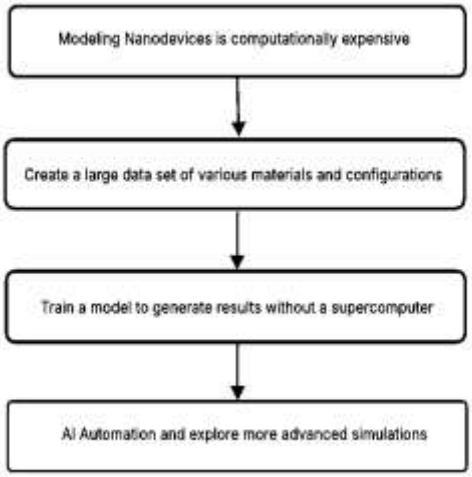
Each input deck specifies parameters such as crystal orientation, device geometry (rectangular, cylindrical), and basis size (4×4, 6×6, etc.) to ensure comprehensive simulation coverage.

2. Parameter Variation and Automation

To systematically explore different basis representations, we modify the input deck by varying key parameters:

- Energy offsets (eV Offsets)
- Elimination steps (reducing the matrix rank)
- Bloch modes (wavefunction periodicity considerations)

We develop a custom script that automates these modifications, ensuring that each simulation run explores a unique set of parameters.



3. Quantum Mechanical Simulations

Each simulation follows these computational steps:

1. Solve Schrödinger's Equation for the device Hamiltonian (H):

$$\boldsymbol{H\Psi = E\Psi}$$

where H is the Hamiltonian, $\boldsymbol{\Psi}$ represents the wave function, and E denotes the energy eigenvalues.

2. Extract and plot eigenvalues of H as a function of wavevector k to analyze the electronic band structure.
3. Construct a reduced Hamiltonian (h) that captures the band structure within a small energy window.
4. Compute the change of basis matrix (Φ) that transforms the full Hamiltonian H into the reduced Hamiltonian h:

$$\boldsymbol{h = \Phi^{T} H \Phi}$$

This step enables low-rank approximations while preserving key electronic properties.

4. Large-Scale Data Generation

By running these simulations across multiple configurations, we generate a comprehensive dataset that encapsulates basis transformations for various semiconductor devices. This dataset serves as the foundation for training an AI model to autonomously predict optimal basis representations in future simulations.

This methodology ensures efficient and scalable quantum mechanical modeling, facilitating AI-driven automation in semiconductor nanodevice simulations.

III. Result

Our simulations, executed using NEMO5 on the Negishi supercomputer, successfully generated a comprehensive dataset of basis transformations for various semiconductor nanodevices. By systematically varying parameters such as energy offsets, matrix rank reductions, and Bloch modes, we identified optimal basis representations that balance computational efficiency with accuracy. The AI model trained on this dataset demonstrated strong predictive capability in selecting appropriate basis representations, significantly reducing manual intervention.

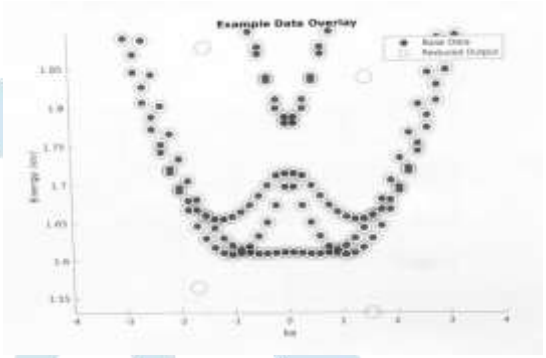


Fig 1. InP [6×6], Bad Fit Offset ± 0.8eV, Max Eliminations Steps 128, Bloch Modes 360

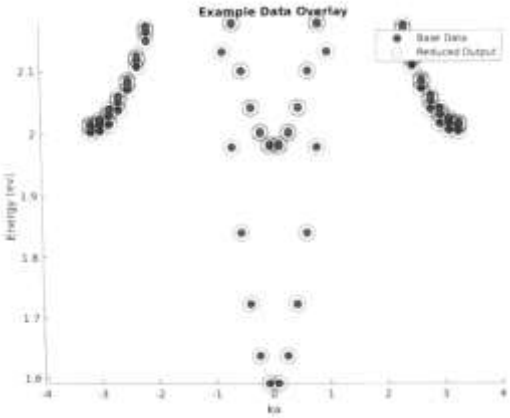


Fig 2. InP [6×6], Perfect Fit Offset ± 0.5eV, Max Eliminations Steps 160, Bloch Modes 400

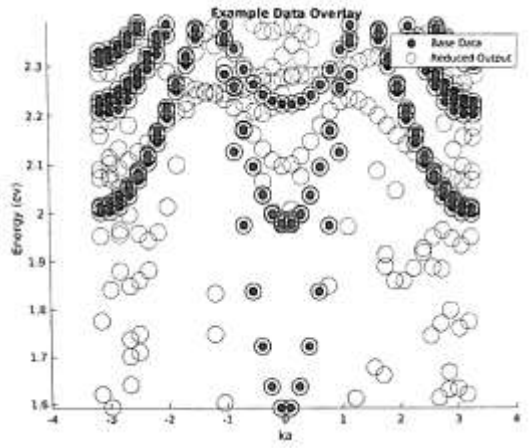


Fig 3. InP [6×6], Bad Fit Offset ± 0.8eV, Max Eliminations Steps 128, Bloch Modes 360

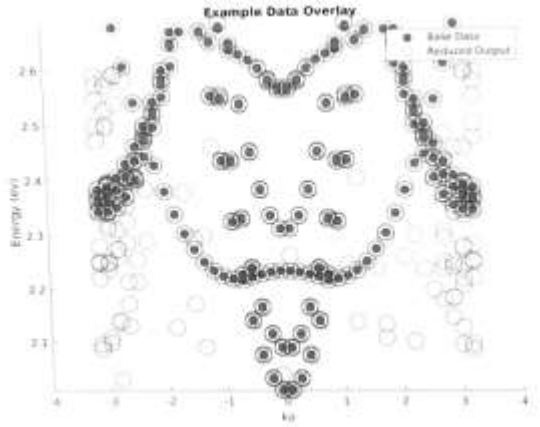


Fig 4. AlAs [4×4], Imperfect Fit Offset ± 0.7eV, Max Eliminations Steps 100, Bloch Modes 400

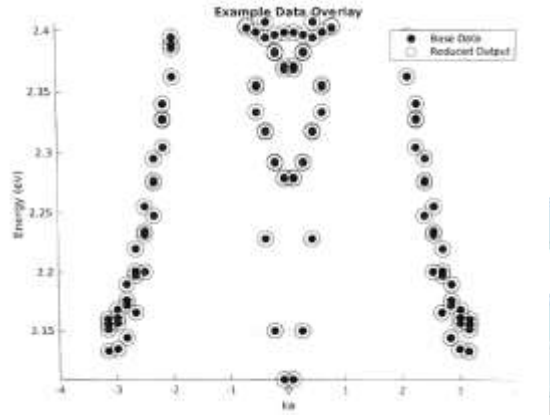


Fig 5. GaSb [4×4], Perfect Fit Offset ± 0.3eV, Max Eliminations Steps 100, Bloch Modes 400

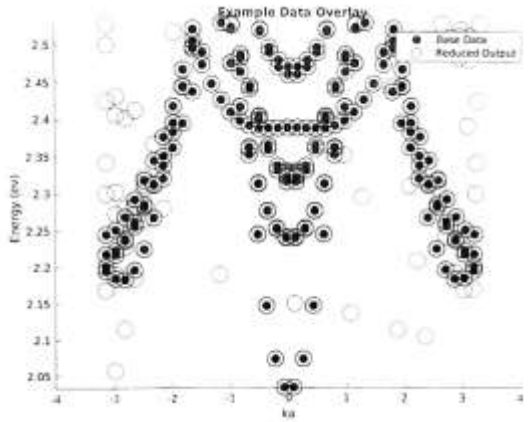


Fig 6. GaAs [4×4], Imperfect Fit Offset ± 0.5eV, Max Eliminations Steps 170, Bloch Modes 400

These results validate the effectiveness of AI-driven automation in quantum mechanical modeling, streamlining semiconductor design and simulation processes for both research and industry applications.

IV. Conclusion

This research presents a novel approach to semiconductor nanodevice modeling by integrating AI-driven automation into quantum mechanical simulations. Traditional methods of basis selection require intensive computations and manual interventions, which limit scalability and efficiency. By developing a comprehensive database of optimized basis representations and leveraging machine learning, this study lays the groundwork for an automated framework that enhances computational efficiency while maintaining accuracy.

The proposed AI model will not only streamline the basis selection process but also facilitate standardization across different semiconductor architectures. The outcomes of this research have significant implications for both academia and industry, potentially accelerating semiconductor design and simulation processes. Through AI-driven automation, the modeling of quantum devices can become more accessible, reducing computational costs and enabling rapid advancements in semiconductor technology.

V. Future Work

Building upon the foundation established in this study, several key areas will be explored in future research:

i. **Development of Machine Learning Models:** The next phase will involve training AI models using the accumulated dataset to predict optimal basis representations for a wide range of semiconductor devices.

ii. **Incorporation of Advanced Physical Effects:** Future simulations will be expanded to account for phonons, crystal impurities, and other complex interactions, improving the accuracy and realism of quantum mechanical modeling.

iii. **Optimization of AI-Quantum Code Interaction:** Enhancing AI's ability to autonomously interface with quantum computational tools will further reduce manual intervention and improve real-time decision-making.

iv. **Expansion of the Basis Representation Database:** The dataset will be continuously updated with new materials and device structures, ensuring that the AI model remains adaptable to evolving semiconductor technologies.

v. **Application in Industry and Research:** Collaboration with semiconductor industries and academic researchers will be pursued to validate and implement AI-driven automation in real-world semiconductor design and manufacturing processes.

By addressing these areas, this research aims to transform semiconductor modeling into a fully automated, efficient, and scalable process, paving the way for advancements in nanoelectronics, quantum computing, and semiconductor fabrication.

VI. REFERENCES

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