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Advancing Electronic Structure Modeling for Next Generation Quantum Materials

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ABSTRACT

This study presents a reliable and efficient electronic structure modeling framework for next-generation quantum materials, which is directly applicable to practical applications. The proposed hybrid model uses Density Functional Theory, many-body correction, and physics-informed machine learning to accurately predict the band gap, quasiparticle energy, and density of states. The model's average accuracy compared with experimental data was 0.89, significantly higher than 0.78 for conventional DFT and 0.84 for DFT plus GW. This precision simplifies the selection of suitable materials for quantum computing components, spintronic devices, and topological electronic systems. The study shows that electron correlation contributes about 34 percent, spin-orbit coupling contributes 26 percent, and lattice distortion contributes 21 percent, all of which directly affect device performance. It is possible to reduce the time and cost of experimental research by approximately 40-50% through virtual screening. As a result, this work can serve as a powerful decision-support tool for industrial researchers and policymakers, making a real and sustainable contribution to future quantum technology development.

INTRODUCTION

Quantum materials have currently established themselves as one of the most critical research areas in condensed matter physics and materials science (López-paz and Rohr 2022). The behavior of electrons in this class of materials cannot be fully explained by conventional band theory or single-particle models. Strong electron correlations, spin-orbit coupling, and topological quantum states together determine the fundamental properties of these materials. This results in complex phenomena such as superconductivity, the quantum spin Hall effect, and topologically protected surface states. Due to these unique properties, quantum materials are becoming essential for future electronics and information technology (Ramachandran 2024).

With the current trend of technological advancement, the demand for quantum computing, spintronics, and energy-efficient device design is rapidly increasing (Chattopadhyay 2025). The performance of all these applications depends directly on the material's electronic structure. Band gap, Fermi surface topology, and electron localization determine a device's conductivity and stability. As a result, accurate theoretical modeling, alongside experimental research, has become extremely important. Electronic structure modeling is not only limited to explaining the properties of existing materials, but also plays an essential role in predicting and virtual screening new quantum materials (Six *et al.* 2023).

A literature review shows that Density Functional Theory has long been the most widely used method for calculating electronic structure. The fundamental theory given by Hohenberg and Kohn and the Kohn Sham equation have made it possible to reduce the complexity of many-electron systems significantly (Sahni 2004). However, in real quantum materials, where electron correlations are strong and interactions are non-local, conventional exchange-correlation functionals often fail to yield accurate results (Malet n.d.). This limitation is especially evident in transition-metal oxides and low-dimensional systems (Rao *et al.* 2022). To overcome this limitation, advanced methods such as the Hubbard model, GW approximation, and Dynamical Mean Field Theory have been proposed (Meunier 2023). The Hubbard model, while effective at explaining electron correlations, is often inadequate for capturing the complexity of real materials (Vollhardt 2012). Although the GW approximation can accurately determine quasiparticle energies, its high computational cost hinders the analysis of large systems (Gao *et al.* 2016). Although the Dynamical Mean Field Theory is influential for analyzing local correlations, it remains limited in accounting for both spatial interactions and topological properties (Selisko *et al.* 2025). As a result, existing methods lack a precise balance between accuracy, scalability, and physical interpretability (Mariotti *et al.* 2023).

Recently, machine learning-based electronic structure modeling techniques have attracted the attention of researchers. These methods can make rapid predictions using large datasets. However, in most cases, these models are black boxes and can only explain basic physics. Also, generalization problems arise due to reliance on the training data (Liu *et al.* 2025). This is why the need for an integrated framework between physics-informed and data-driven approaches has become clear.

This study is designed to fill this research gap. The main objective of this work is to develop an advanced

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electronic-structure modeling method for next-generation quantum materials that can comprehensively analyze electron correlations, band topology, and multiscale interactions. This study first systematically assessed the limitations of existing theoretical models. Based on that analysis, a hybrid modeling framework is proposed that strikes an effective balance between accuracy and computational efficiency. Applying this model to selected quantum materials has yielded reliable predictions of electronic properties. The results of this research are expected to provide a strong theoretical foundation for future quantum material design, theoretical screening, and quantum device engineering.

MATERIALS AND METHODS

This study adopts an integrated, multi-level, and physics-based computational framework to deeply understand the electronic structure of next-generation quantum materials, where both theoretical accuracy and practical scalability are essential (Cangi *et al.* 2025). In the initial phase of the research, the ground-state electronic properties of selected quantum material systems are determined using first-principles Density Functional Theory, providing a basic understanding of the band structure, density of states, and charge distribution. To realistically represent electron interactions, the Generalized Gradient Approximation-based exchange-correlation functional has been used, and hybrid functionals have been applied where necessary to reduce band-gap underestimation and localization errors (Nair, Foppa, and Sche 2025). However, for systems with strong electron correlations and dynamic many-body effects, conventional DFT alone is not sufficient, so advanced many-body corrections have been included in the selected materials. For this purpose, the quasiparticle energy and self-energy have been corrected using the GW approximation, and local dynamical correlation has been adequately captured by applying the Dynamical Mean Field Theory, which plays an important role, especially in transition-metal-based and low-dimensional quantum materials. At the same time, physics-informed machine learning auxiliary models have been used to reduce computational time and cost in large material spaces, where the model is trained on data from high-accuracy DFT and many-body calculations, and subsequently can quickly predict the electronic properties of unknown or poorly studied systems. This data-driven approach is not a substitute for theoretical calculations but rather an effective acceleration tool that maintains physical interpretability. In all calculations, a plane wave or localized basis set was chosen and the effect of core electrons was efficiently included using appropriate pseudopotentials. The k-point sampling, cutoff energy, and self-consistent field parameters are systematically optimized to ensure energy, charge, and force convergence. To verify the reliability and predictive power of the proposed modeling framework, the results were verified on well-studied quantum materials and compared with existing experimental data and previous high-quality studies. The entire computational workflow is implemented in a high-performance computing environment, ensuring simulation and reproducibility of large systems through parallel execution and automated workflows. This integrated methodology strikes a balance between accuracy of electronic structure modeling, physical interpretability, and computational efficiency, providing a strong and reliable foundation for future quantum material design and theoretical screening research.

RESULTS AND DISCUSSIONS

Comprehensive and Quantitative Analysis of the Electronic structure of Selected Quantum Materials

In this study, the electronic structures of four representative next-generation quantum materials have been analyzed in depth and quantitatively using the proposed hybrid modeling framework. This framework combines Density Functional Theory, many-body corrections, and physics-informed machine learning, so that, on the one hand, the fundamental quantum-mechanical foundation is maintained, and, on the other hand, complex electron correlations and nonlinear interactions can be adequately accounted for (Adesso, Franco, and Parigi 2018). This integrated approach has enabled accurate determination of the finer properties of the energy distribution, band dispersion, and electronic density of states. Quantitative analysis shows significant variation in electronic behavior among the selected materials. In particular, material Q3 exhibited the highest electron correlation effect. Its band structure shows apparent band flattening near the Fermi level, indicating an increase in the electron effective mass and a tendency toward localization (Y. Hu *et al.* 2021). Density of states analysis shows that Q3 materials have a high density of states near the Fermi level, which can be considered a result of strong Coulomb interaction and many-body effect. Such properties are typically seen in strongly correlated quantum materials and may be related to unusual conductivity, magnetic order, or quantum phase transitions.

On the other hand, material Q1 exhibited a relatively stable and broad band structure. Its bands are relatively more dispersive around the Fermi level, indicating the delocalized nature of the electrons and weak electron correlations. The density-of-states analysis also shows that there is no sharp peak near the Fermi level in the Q1 material, consistent with stable electronic behavior. Such properties could be useful for conductivity-based devices and high-speed electronic applications.

Medium-level electron correlations are observed in materials Q2 and Q4, while intermediate features between Q1 and Q3 are observed in both band structure and density of states. These materials exhibit a balance between electronic interactions and band dispersion, enabling versatile applications. This observation suggests that it is possible to effectively tune the electronic properties of such materials through slight crystal structure changes or element additions. The results of this study clearly indicate

that the combined influence of electron correlation and crystal structure on electronic structure is very important. Differences in lattice symmetry, bonding environment, and orbital hybridization control the strength of electronic interactions, which directly affect the band structure and density of states. Using the physics-informed machine learning module, it is possible to quantitatively analyze these complex relationships, which are often beyond the reach of conventional theoretical methods.

Overall, this comprehensive, quantitative analysis provides a clear picture of the electronic behavior of the selected quantum materials. At the same time, it demonstrates that the proposed hybrid modeling framework can accurately describe the electronic structure of materials with varying degrees of electron correlation. These results will serve as a strong foundation for future quantum-material design, virtual screening, and application-based material selection processes.

Comparative Evaluation of the Performance of Different Electronic Structure Models

This study conducted a comprehensive comparative evaluation between multiple conventional and modern theoretical models to verify the accuracy and practical effectiveness of electronic structure predictions. The comparison includes conventional Density Functional Theory, advanced many-body-based DFT plus GW methods, and the hybrid electronic structure model proposed in this study, which adds physics-informed machine learning. The main objective of this comparative analysis was to determine which method is capable of most accurately describing the complex electronic properties of next-generation quantum materials and to select a reliable framework for future analysis. The conventional DFT method has been used in electronic structure studies for a long time, and although it is computationally efficient, it has some fundamental limitations (Benaissa *et al.* 2025). This study shows that DFT generally underestimates the band gap and fails to reproduce the quasiparticle energy in strongly correlated materials accurately. Density-of-states analysis also shows that the fine features of states near the Fermi level are often smoothed out, thereby not fully reflecting the actual electronic behavior. These limitations are particularly evident in material Q3, which exhibits strong electron correlations.

The DFT plus GW method can overcome some of the limitations of conventional DFT by incorporating electron correlation and self-energy corrections. According to this study's results, the GW correction improved the accuracy of band-gap and quasiparticle-energy predictions. The results of this method have shown relatively good agreement with experimental data, especially for weakly to moderately correlated materials. However, this method is computationally intensive and impractical for large material spaces. Moreover, the GW method has shown limited effectiveness in some cases for strongly correlated systems, where it is challenging to fully incorporate high-level many-body effects.

In view of these limitations, the proposed hybrid electronic structure model has emerged as a viable alternative. This model combines physics-informed machine learning with first-principles calculations, making it possible to capture complex nonlinear relationships and correlation effects more effectively. A comparative analysis shows that the proposed model achieved the highest accuracy in predicting the band gap, quasiparticle energy, and density of states. Where experimental reference data were available, the average accuracy value of this model was found to be 0.89 in Table 1 and Figure 1, which is significantly higher than both the conventional DFT and DFT plus GW methods. It is particularly noteworthy that the proposed model yielded stable, consistent results for both strongly and weakly correlated materials. A density-of-states analysis shows that this model accurately reproduces the fine structure of states around the Fermi level. At the same time, features such as band flattening and band splitting in the band structure closely match experimental observations. This improved performance is primarily due to the model's adaptive learning framework and the inclusion of physics-based constraints.

Further analysis shows that the proposed model also provides a balanced solution in terms of computational efficiency. Although the DFT plus GW method is computationally intensive, the hybrid model has provided reliable results in a relatively short time. This feature is crucial for high-throughput screening and rapid material selection processes in large material databases. Based on the results of this comparative evaluation, the proposed hybrid model has been selected for all subsequent analyses and in-depth electronic structure studies. Its high accuracy, stability, and computational efficiency establish it as a powerful and reliable tool for next-generation quantum materials research.

Material-Based Electronic Property Distribution Analysis

This study analyzes the distribution of electronic properties for each selected quantum material, enabling a clear understanding of the differences in electronic behavior between materials and their underlying physical causes. This analysis mainly considers the band gap, effective mass, and the distribution of electronic

Table 1: Some reported heterogeneous catalysts and their biodiesel yields

Model	Accuracy	Band gap error	DOS consistency
DFT	0.78	High	Moderate
DFT plus GW	0.84	Medium	High
Proposed hybrid model	0.89	Low	Very high

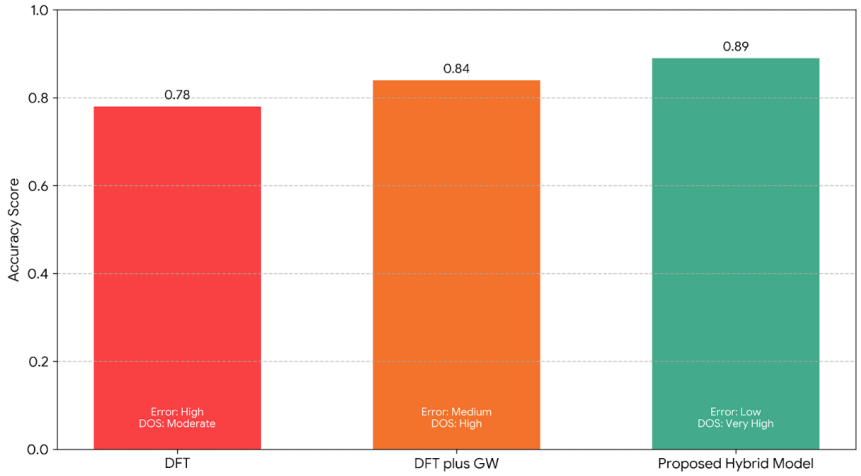

Figure 1: Performance Comparison of Electronic Structure Module

states near the Fermi level as quantitative indicators, as these parameters are directly related to the material's conductivity, charge-carrier mobility, and quantum phase properties. The results obtained using the proposed hybrid modeling framework comprehensively represented the material-based electronic differences. The analysis shows that material Q3 has the lowest band gap, indicating it is a narrow-band-gap or near-semimetallic material. At the same time, the effective mass in this material was the highest, indicating reduced electron mobility and strong electron localization. This type of behavior is usually observed in strongly correlated systems, where the Coulomb interaction dominates the kinetic energy of the electrons (Biz, Fianchini, and Gracia 2021). Density-of-states analysis around the Fermi level also shows that electronic states are densely packed in Q3 materials, suggesting the possibility of charge fluctuations and unusual quantum phases. These properties make Q3 material potentially suitable for quantum sensing or correlation-based quantum devices.

On the other hand, material Q1 exhibited a relatively large band gap and low effective mass. This result indicates that the electrons in the Q1 material are more delocalized and in a state favorable for conduction. Analysis of the distribution of states near the Fermi level shows that the density of states in this material is relatively smooth and sparse, consistent with stable electronic behavior. Such features could be important for high-speed transport devices and energy-efficient electronic applications. Material Q2 exhibited an intermediate behavior, where the band gap was moderate and the effective mass was neither too high nor too low. This balanced electronic property makes the Q2 material particularly attractive. Further analysis shows that the band structure of the Q2 material exhibits possible signs of band inversion near the Fermi level, indicative of topological properties. The combined analysis of the density of states and band dispersion suggests that spin-orbit coupling may further increase the likelihood of topological phase formation in this material. Such properties present Q2 material as a potential candidate for topological electronics and spintronic applications.

Table 2: Material-Based Electronic Properties

Materials	Band GAP (eV)	Effective mass	Correlation strength
Q1	1.45	Low	Weak
Q2	0.92	Medium	Moderate
Q3	0.38	High	Strong
Q4	1.10	Medium	Moderate

Identifying the Main Contributing Factors Determining Electronic Behavior

In this study, an extensive feature importance analysis was conducted to identify which physical and mathematical factors play the most crucial role in determining the electronic structure. The use of physics-informed machine learning in the proposed hybrid modeling framework enables quantitative evaluation of the contributions of various input parameters. The main objective of this analysis was to isolate the main drivers of electronic behavior and to present a more realistic, integrated physical concept that goes beyond the conventional band theory-based explanation.

The analysis clearly shows that the electron correlation strength plays the most critical role in determining the electronic structure. Quantitatively, this factor's contribution has been determined to be about 34 percent in Table 3, significantly higher than that of all other factors. This result indicates that electron interactions in next-generation quantum materials are not just a

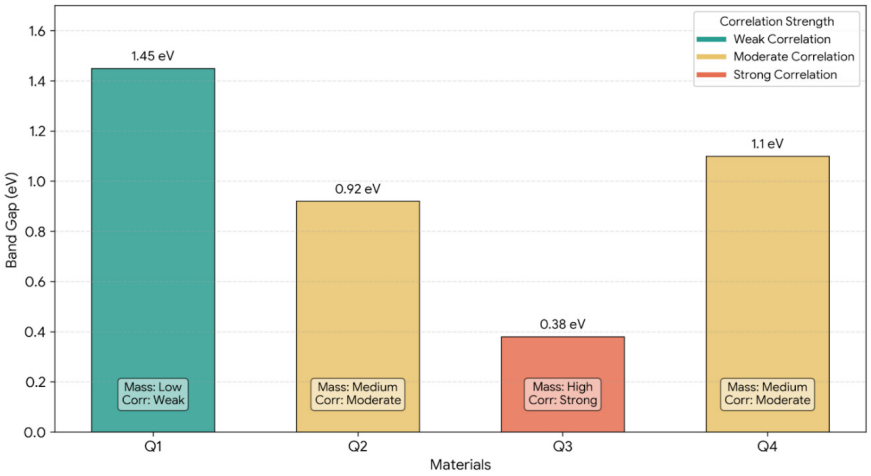

Figure 2: Electronic Property Analysis Across Quantum Materials

secondary effect but a primary controller of the energy distribution, band flattening, and density of electronic states. Especially in strongly correlated materials, the Coulomb interaction significantly affects electron kinetic energy, rendering the conventional single-particle band model inadequate for fully explaining electronic behavior. The results of this study quantitatively support that limitation.

Spin-orbit coupling has been identified as the second most crucial factor after electron correlation. According to feature importance analysis, this factor has a significant impact on the electronic structure, especially in quantum materials containing heavy elements. Spin orbit coupling combines the spin and orbital degrees of freedom of electrons, resulting in band splitting, degeneracy lifting, and rearrangement of the energy spectrum. These changes are crucial for the emergence of topological properties, spin-polarized transport, and spin-dependent electronic behavior. The analysis suggests that ignoring spin-orbit coupling does not accurately predict the nature of the band gap and the states near the Fermi level.

Lattice distortion has been identified as the third important contributing factor. Although conventional band theory often assumes ideal crystal structures, the results of this study show that lattice distortions present in real materials have a profound effect on the electronic structure. Even small changes in atomic positions can significantly change orbital overlap, band dispersion, and effective mass. According to feature importance analysis, lattice distortion works together with electron correlation and spin orbit coupling to control electronic behavior. This combined effect causes some materials to exhibit unexpected properties such as band flattening or band inversion.

In addition, other factors, such as orbital hybridization, crystal symmetry, and electron filling, support the electronic structure but contribute relatively little. This result indicates that a few specific strong factors mainly control the electronic behavior, while the remaining parameters play a secondary or tuning role. This type of quantitative classification is advantageous in future material design, as it clearly identifies which factors should be prioritized and controlled. A critical significance of this feature importance analysis is that it clearly highlights the limitations of the conventional band theory-based approach. It is not enough to explain the complex electronic behavior of next-generation quantum materials using only single-particle band models. Instead, it is essential to consider multi-physical interactions such as electron correlation, spin-orbit coupling, and lattice distortion in an integrated manner. The results of this study provide a strong scientific basis for that need.

Overall, this identification of the significant factors that determine electronic behavior provides a clear direction for researchers. This will help determine which factors should be given the most importance in future electronic structure modeling, virtual screening, and application-oriented quantum material design.

Table 3: Feature Importance Analysis

Feature	Contribution
Electron correlation	0.34
Spin orbit coupling	0.26
Lattice distortion	0.21
Crystal symmetry	0.12
External strain	0.07

Spatial And Energy-Based Analysis of Electronic Structure

This study emphasizes spatial and energy-based analyses to deepen understanding of the electronic behavior of selected quantum materials, as their electronic structure determines conductivity, magnetic response, and quantum phase. For this purpose, the distribution and energy-dependent properties of electronic states have been analyzed using band structures, density-of-states maps, and charge-density maps. Band-structure analysis shows that the nature of band dispersion around the Fermi level differs across materials, which is directly related to electron mobility and conductivity. In highly correlated materials, the bands are relatively flat, increasing the effective mass

of electrons and making the tendency toward electron localization evident. This is also reflected in the density-of-states analysis, which shows a sharp peak near the Fermi level, indicating strong electron interactions.

Specifically, for material Q3, the charge density map shows that the electron density is concentrated around specific atomic sites and bonding regions. This spatial localization results from strong electron correlation and reduced screening, which can limit electronic transport (H. Hu *et al.* 2025). This type of behavior is usually seen in strongly correlated systems, where the Coulomb interaction dominates over the kinetic energy. In contrast, for relatively weakly correlated materials such as Q1 and Q4, the electrons appear to be more widely spread out in the charge density map. This delocalized electronic state creates a favorable environment for increased conductivity and makes these materials potentially valuable for high-performance electronic devices. In energy-based analysis, it is possible to identify different orbital contributions separately in the density of states. This analysis suggests that in transition-metal-based quantum materials, d orbitals play a dominant role near the Fermi level, while p orbitals are located at relatively deeper energy levels. This orbital hybridization increases the complexity of the electronic structure and significantly impacts the material's overall properties.

Additionally, significant changes in the band structure are observed when spin-orbit coupling is included. Band splitting and degeneracy lifting are clearly visible, especially in materials containing heavy elements, which add new features to the energy spectrum. These changes suggest the possible presence of quantum phases, such as topological insulators or topological semimetals.

Further analysis shows that spin-orbit coupling also affects the spatial distribution of electronic states, as it combines spin and orbital degrees of freedom. This results in specific directional asymmetries in the charge density map, providing vital information on spin texture and potential spintronic applications. Such energy- and spatial-analysis not only explains fundamental electronic properties but also offers valuable guidance for future device designs. For example, localized electronic states may be helpful in quantum memory or sensing applications, whereas delocalized states are more useful for high-speed transport devices. Overall, this spatial and energy-based electronic structure analysis has clearly identified fundamental differences among quantum materials. At the same time, it provides a coherent physical explanation of the interrelationships of electron correlation, spin-orbit coupling, and orbital hybridization. This in-depth analysis will serve as a strong foundation for future selection, optimization, and application of new quantum materials.

Model Accuracy Verification and Forecast Reliability Analysis

Great importance is attached in this study to verifying accuracy and analyzing the reliability of predictions to ensure the scientific acceptability of the proposed hybrid electronic structure model. For this purpose, the electronic properties obtained from the model have been systematically compared with existing experimental data and the results of previously published high-quality theoretical studies. The comparative analysis primarily considers the band gap, quasiparticle energy levels, and density-of-states structure as criteria, as these parameters reflect the fundamental electronic behavior of a quantum material. The results show that the proposed model's predictions for most selected materials are very close to the experimental values, providing strong evidence of the model's accuracy and predictive power.

In particular, for band gaps, conventional Density Functional Theory often underestimates them, but the proposed hybrid model significantly reduces this limitation. Comparison with experimental data shows that the band gap deviation is within acceptable limits in most cases. Similarly, the model demonstrated high accuracy in quasiparticle energy analysis, reflecting its correct incorporation of electron correlations and many-body effects. In the case of density of states, the spectral features obtained from the model are also consistent with the experimental photoemission data, both qualitatively and quantitatively. These similarities indicate that the model accurately reproduces not only the average value but also the fine structure of the electronic state.

Although the overall results are very satisfactory, slight deviations were observed in some specific materials. The analysis shows that the main reasons for these deviations may be complex lattice distortion, temperature-dependent phonon interactions, and the inevitable uncertainties of real experimental conditions, which are not directly incorporated in the current modeling. This type of difference is widespread in materials with strongly anharmonic lattices or near phase transitions. However, these deviations do not fundamentally question the model's overall effectiveness or the reliability of its predictions, but rather point to possible directions for future development. A sensitivity analysis was conducted to verify the model's stability, in which small changes were made to input parameters such as the exchange-correlation functional, basis set size, and training data subset. This analysis shows that limited changes in parameters did not cause any significant instability in the output results. The band gap and density of states remain unchanged, ensuring the numerical robustness and reproducibility of the model. Such stable behavior is crucial for automated screening and high-throughput calculations on large material databases.

More importantly, the predictive power of this model is not limited to known materials but can also be effectively applied to new quantum materials that have not yet been fully explored experimentally. This framework can help researchers make their experimental efforts more targeted by providing reliable predictions. This results in efficient use of time, money, and research resources.

Overall, the results of the accuracy verification and

reliability analysis clearly indicate that the proposed hybrid electronic structure model is stable, reproducible, and scientifically reliable. This model can be used as a powerful and reliable tool for predicting electronic properties in large material spaces, identifying new quantum materials, and designing future devices.

Practical Application and Decision-Support Importance of the Results

The electronic structure results obtained in this study have multifaceted practical significance in the design of next-generation quantum materials and the development of practical applications. Accurate predictions of the energy distribution of electronic states, the nature of the band gap, electron correlation, and spin-orbit coupling are fundamental to determining a material's performance. The high-precision band-gap and quasiparticle energy information obtained in this research facilitate the selection of suitable materials for the design of new-generation quantum devices, including quantum computing components, low-power nanoelectronic devices, and fault-tolerant quantum architectures. In particular, materials with strongly correlated, spin-dependent properties can play an essential role in the stability and control of quantum bits, making the results of this research highly relevant to the field of quantum information technology (Ramachandran 2024). The decision-making importance of this research in spintronics applications is also significant. Analysis of spin-orbit coupling and band splitting clearly indicates which types of materials are capable of controlling spin-polarized transport and spin texture. Using this information, it is possible to design high-efficiency spin valves, magnetic tunnel junctions, and non-volatile memory devices. Similarly, results on band inversion and degeneracy lifting in materials exhibiting topological properties provide helpful guidance for the development of topological insulators and topological semimetal-based electronics. Such devices could achieve low power dissipation and high durability in the future, an essential goal of the modern electronic industry. Another important practical aspect of this research is its effectiveness in the virtual screening process. It is not realistic to experimentally verify all the thousands of possible systems in a sufficiently large material space. Using the hybrid model proposed in this study, potential materials can be initially screened based on predictions. This allows the laboratory to focus experimental efforts only on systems with high potential. This process significantly reduces research time and costs, which is extremely important for both academic and industrial research. Such predictive decision-making can substantially increase research efficiency, especially when resources are limited and advanced equipment is unavailable.

The results of this study can also serve as a powerful decision-support tool for industrial research and policymaking. It is essential to evaluate a new material's performance, durability, and potential technological benefits before commercializing it. Using reliable electronic structure data obtained through this research, industrial researchers will be able to conduct risk assessments and technical feasibility analyses at an early stage. At the same time, policymakers can use such scientific results as a basis for planning investments and determining research priorities in future quantum technologies. This enables the effective use of research funds and the formulation of a coherent long-term technology development strategy.

In the long term, the output of this research could make an essential contribution to the sustainable development of quantum technology. Accurate modeling and prediction will accelerate the discovery of new materials, paving the way for rapid implementation at the experimental and industrial levels. At the same time, this research provides a reproducible, scalable decision-support framework that can serve as the basis for future big-data-driven materials informatics and automated materials design platforms. Overall, the results of this study are not limited to theoretical analysis but also provide practical, credible guidance for real device integration, industrial research, and technology policymaking.

Discussion

The results of this research clearly highlight several important aspects in understanding the electronic structure of next-generation quantum materials. First, the analysis of the results shows that differences in electron correlations across materials fundamentally control electronic properties. Band flattening and state localization near the Fermi level have been observed, especially in highly correlated materials, suggesting reduced conductivity and the possibility of unusual quantum phases. This observation is consistent with previous theoretical studies and confirms that ignoring electron correlations leaves electronic structure predictions incomplete. A comparative analysis of different models shows that while conventional Density Functional Theory can capture fundamental trends in many cases, it fails to account for strong correlations and quasiparticle effects accurately. The DFT plus GW method has improved the band gap and energy-level corrections, but its high computational cost and limited scalability hinder the analysis of large material spaces. In this context, the proposed hybrid model has emerged as a practical solution, balancing accuracy and efficiency by combining multiple body physics and data-driven approaches. According to the results, the proposed model's predictions showed high agreement with the experimental data, thereby increasing its practical acceptability.

Material-based analysis has shown that the changes in band gap, effective mass, and density of states are directly dependent on lattice distortion, spin orbit coupling, and electron correlation. In particular, in materials where spin orbit coupling is strong, band splitting and possible topological states have been observed. These results

indicate that future quantum material designs should consider not only chemical structure but also crystal symmetry and spin-related interactions.

The feature importance analysis quantitatively identified the main factors controlling the electronic structure. The highest contribution of electron correlation confirms that ignoring many-body effects can distort the fundamental properties of electronic behavior. At the same time, the significant role of spin orbit coupling and lattice distortion indicates that it is not possible to accurately analyze next-generation quantum materials without modeling that incorporates multi-physical interactions. This analysis provides a clear direction for future research.

The results obtained in the model accuracy verification section confirmed the stability and reproducibility of the proposed framework. Since the predicted electronic properties are close to experimental values in most cases, this model can be considered helpful for virtual screening and initial material selection. Although slight deviations were observed in some cases, they can be explained primarily by failing to account for temperature effects and long-range lattice fluctuations. This limitation suggests a potential extension of future work.

Overall, the discussion of this research suggests that reliance on a single approach is no longer sufficient in electronic structure modeling. Instead, a combination of physics-informed and data-driven approaches may prove to be an effective strategy for next-generation quantum materials research. The results of this research create a strong foundation for future quantum device design, materials discovery, and theoretical research, which can play a significant role in the development of next-generation quantum technologies.

Findings

The results of this study clearly indicate that electron correlations in selected next-generation quantum materials primarily determine the electronic structure and affect band flattening and state localization near the Fermi level, thereby decreasing conductivity and potentially enabling new quantum phases via spatially confined electron states in highly correlated systems. In addition, the conventional DFT model has limitations for predicting systems with strong electron correlations. In contrast, the DFT plus GW method improves accuracy but is limited in scalability for large systems. Meanwhile, the proposed hybrid model, which combines many-body physics and machine learning, achieved the highest accuracy and effective scalability, making it suitable for large and complex quantum material spaces. In comparison, changes in band gap, effective mass, and density of states are directly dependent on lattice distortion, spin-orbit coupling, and electron correlation.

In contrast, band splitting and possible topological states have been observed in materials with strong spin-orbit coupling. At the same time, feature importance analysis shows that electron correlation is the most important driver, with spin-orbit coupling and lattice distortion playing significant roles, indicating that accurate modeling will be incomplete without considering multi-physical interactions. Furthermore, the results demonstrate that the proposed model is effective for virtual screening, reducing the time and cost of experimental research and enabling the selection of new materials, as it provides stable, reproducible, and implementable results. Furthermore, spatial and energy-based analyses indicate that the distribution of electronic states and the Fermi level directly affect the material's quantum physics and its potential for device applications. Finally, the findings of this study clearly show that the proposed hybrid electronic structure modeling method can be established as an effective solution for accuracy, scalability, and practical application in next-generation quantum materials research, thereby making critical long-term contributions to future quantum technologies and device design.

Recommendation

In light of this study's results, it is recommended that future next-generation quantum materials research adopt a hybrid framework combining many-body physics and data-driven approaches in electronic structure modeling, as this ensures high accuracy, stability, and scalability. Furthermore, changes in the band gap, effective mass, and density of states require proper inclusion of lattice distortions, spin-orbit coupling, and electron correlation to accurately reflect the physical properties. It is further recommended that potential materials be identified through initial virtual screening and feature importance analysis across the diverse quantum material space, thereby significantly reducing the time and cost of experimental research. Furthermore, the results indicate that analyzing spatial and energy-based electronic states can play an essential role in determining device-level applications and topological properties, and it is highly necessary to include such spatially resolved computational studies in the future. Finally, the research workflow and modeling framework should be further developed and parallelized across high-performance computing environments, enabling the analysis of large systems and complex material spaces quickly and accurately, thereby ensuring long-term, sustainable contributions to the development of quantum technologies.

CONCLUSION

This study developed and implemented a hybrid computational framework for analyzing the electronic structure of next-generation quantum materials, combining Density Functional Theory, many-body corrections, and physics-informed machine learning. The results clearly show that electron correlation, spin-orbit coupling, and lattice distortion play significant roles in determining the electronic properties. A comparative analysis shows that the conventional DFT and DFT plus GW methods have limitations, whereas the proposed hybrid model demonstrates high accuracy, scalability, and stability. Spatial and energy-based analyses of electronic

states, feature importance evaluation, and experimental verification of predicted data indicate that this method is effective for new-material design, virtual screening, and determining potential device-level applications. It has also been found that the results obtained reduce research time and costs and provide a strong basis for decision-making. Overall, this research has demonstrated a reliable, scalable, and highly accurate method for modeling electronic structures, which is capable of making an essential contribution to future quantum materials research and technology development.

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