Review

State of the Art and Future Perspectives of DFT Applications in Functional Materials Analysis in Tajikistan

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State of the Art and Future Perspectives of DFT Applications in Functional Materials Analysis in Tajikistan

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Abstract

This review highlights the current progress and future prospects of applying Density Functional Theory (DFT) for studying functional materials in Tajikistan. DFT has become a cornerstone of modern materials science, allowing accurate modeling of electronic structures, optical properties, and thermodynamic stability of compounds relevant to energy and optoelectronic applications. The article outlines methodological advances, major areas of application including kesterites, perovskites, and transition-metal oxynitrides, and the formation of a DFT research school. The discussion emphasizes the integration of DFT with experimental techniques and machine learning, as well as the strategic role of computational materials science in advancing sustainable energy technologies and scientific independence in Tajikistan.

Keywords: density functional theory; functional materials; photovoltaics; perovskites; kesterites; oxynitrides; tajikistan; phonons; transport; machine learning

Introduction

Density Functional Theory (DFT) is one of the key instruments of modern materials science. This method makes it possible to describe electronic structure and interatomic interactions with quantum accuracy, providing a deep understanding of the physical mechanisms that underlie the properties of functional materials. Owing to its strong predictive power, DFT plays a central role in the study of semiconductors, perovskites, kesterites, oxides, and oxynitrides used in solar cells, light-emitting diodes, photocatalysts, and other energy-efficient systems [1–3].

In recent years, Tajikistan has seen notable progress in theoretical approaches and computational methods for the analysis of functional materials. Young researchers in the country actively employ modern DFT tools to model crystal structure, energy bands, optical parameters, and the stability of promising compounds. The use of advanced exchange–correlation functionals such as SCAN, TB-mBJ, and HSE06, as well as the integration of computational packages VASP, WIEN2k, Quantum ESPRESSO, and Phonopy, has enabled high-accuracy descriptions of structural and electronic characteristics across various classes of compounds [4–8]. Particular attention is devoted to semiconductor systems based on group IV–VI elements, where DFT is used for engineering control of the band gap and optimization of optical properties. A number of recent studies have shown that isoelectronic substitution in kesterites of the $Cu_2ZnSn(S,Se)_4$ or $Cu_2Ni(Sn,Ge,Si)Se_4$ type leads to controllable changes in the band gap, which allows the light absorption parameters to be aligned with the solar spectrum and increases energy conversion efficiency. Analyses of the electronic density of states (DOS) and band structures demonstrate that such materials possess direct or quasi-direct transitions, which makes them attractive for photovoltaic applications [9–11].

Research on lead-free perovskites is developing in parallel, where theoretical modeling is used to study geometric stability, the impact of halide substitution, and phase transitions on electronic and optical properties. Calculations have shown that transitions between tetragonal and cubic phases are accompanied by shifts in the Fermi level and changes in the refractive index, which significantly affect

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the efficiency of devices based on perovskite structures. These results create a foundation for the development of environmentally safe photoactive materials with high stability and predictable characteristics [12–14].

Equally important are oxide and oxynitride systems such as ZrO_2, TaON, and $BaNbO_2N$, which are considered promising photocatalysts for hydrogen generation and water treatment. Modeling of surface interactions, phonon properties, and defect formation energies has shown that controlled doping with transition metals can improve visible-light absorption and enhance photocatalytic activity. The DFT studies carried out have explained the mechanisms of water adsorption on oxide surfaces and identified stable configurations of hydroxyl groups, which is important for creating new catalytic coatings and sensor devices [15–17].

In recent times, researchers have also focused on integrating DFT with machine learning methods. This hybrid approach opens the possibility of accelerated property prediction and the selection of promising compounds without performing a complete ab initio recalculation. ML models trained on DFT data demonstrate high accuracy in predicting structural and optical parameters and make it possible to efficiently optimize material compositions for photocatalysis and solar cells [18–20]. Thus, the growth of DFT-oriented research in Tajikistan reflects the increase in the country's scientific potential in quantum materials science. The results of recent years indicate the formation of a stable theoretical school capable of addressing pressing challenges in renewable energy, optoelectronics, and nanotechnology, combining advanced quantum computational methods with applied engineering tasks.

2. Methodological Foundations of DFT and Applied Approaches

The methods of Density Functional Theory form the basis of the overwhelming majority of modern quantum-mechanical studies of solids, nanostructures, and molecular systems. Their use in physics and materials science is due to the fact that DFT makes it possible to compute the electronic structure of many-particle systems with high accuracy, describing fundamental parameters, including the density of states, charge distribution, band gaps, bond strengths, and optical responses, at reasonable computational cost [2, 21, 22]. The theory rests on the Kohn–Sham equations, in which interactions between electrons are approximated through the exchange–correlation functional. The quality and reliability of calculations are to a large extent determined by the choice of this functional, so a significant part of current research is aimed at improving its accuracy. In practice, several major categories of functionals are employed for the analysis of functional materials:

- LDA (Local Density Approximation), a local approximation effective for systems with a uniform distribution of electron density, though it often overbinds and underestimates the band gap [23].
- GGA (Generalized Gradient Approximation), including the PBE (Perdew–Burke–Ernzerhof) parameterization, which provides a better description of weak interactions and structural properties, but may still underestimate band-gap values [24].
- meta-GGA and SCAN (Strongly Constrained and Appropriately Normed), advanced approximations that more accurately reproduce thermochemical and structural properties and are more robust to systematic correlation errors [25].
- TB-mBJ (Tran–Blaha modified Becke–Johnson), a potential that substantially improves the accuracy of band-gap descriptions, especially for semiconductors and insulators, at relatively low computational cost [26].
- HSE06 and other hybrid functionals, which combine the contribution of exact Hartree–Fock exchange with DFT correlation, providing the most accurate description of band structure and optical transitions, while requiring significant resources [27].

For practical implementation of DFT approaches, Tajik researchers actively use high-performance software packages that solve the Kohn–Sham equations in various representations of the wave function. These include VASP (Vienna Ab Initio Simulation Package), WIEN2k, Quantum ESPRESSO, CASTEP, Phonopy, and BoltzTraP, each of which has its own advantages and domain of

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application [28–30].

VASP is based on the projector augmented-wave method and plane waves, which makes it convenient for modeling crystalline systems and for studying surfaces, defects, and adsorption processes. WIEN2k implements the linearized augmented plane-wave method and provides exceptionally high accuracy in calculating electronic density and band characteristics, especially when studying complex semiconductor systems. Quantum ESPRESSO and CASTEP are widely used for geometric optimization and phonon calculations, while Phonopy is employed to analyze vibrational spectra, thermodynamic functions, and dynamic stability. BoltzTraP, in turn, makes it possible to compute transport parameters, including carrier mobility, thermoelectric coefficients, and conductivity, based on band-structure data [31, 32].

In recent studies by Tajik research groups, these tools have been applied to comprehensive investigations of the energetic stability and optical properties of kesterites, perovskites, and oxide and oxynitride materials. Calculations were carried out using carefully selected parameters, including Monkhorst–Pack meshes with high k-point density, energy cutoffs of 400–600 eV, and strict convergence criteria for energy in the range of 10^{-5} to 10^{-6} eV. This approach yielded reproducible results that agree well with experimental data, confirming the reliability of the chosen methodologies [33, 34]. Phonon calculations are widely used to describe dynamic properties and phase stability. Analyses of phonon dispersion and density of states make it possible to identify soft modes that indicate structural transitions or lattice instability. Such studies have been performed for perovskite systems $CsSnI_3$ and $CsPbBr_3$, as well as for oxynitrides TaON and $BaNbO_2N$. In combination with the computation of Gibbs and Helmholtz thermodynamic potentials, this makes it possible to predict temperature-dependent behavior and the ranges of phase stability [35–37].

Particular attention is also paid to calculations of optical and electronic properties. The use of averaged dielectric functions and frequency-dependent refractive indices makes it possible to determine the nature of optical transitions and the range of spectral absorption. Analyses of the frequency dependencies of $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$, as well as reflectivity, absorption coefficient, and electron energy-loss function, provide valuable insights into a material's potential for application in photovoltaics and photocatalysis [37–39].

Taken together, the accumulated methodological experience attests to the maturity and technological competence of the national DFT-modeling school, which is capable of addressing world-class challenges in functional materials, optoelectronics, and renewable energy.

3. Application of DFT in Research on Functional Materials

The application of Density Functional Theory in Tajik research centers in recent years covers a wide range of tasks related to the design and analysis of functional materials for energy, optoelectronics, and photocatalysis. Studies conducted in the research laboratories of the National Academy of Sciences of Tajikistan, in universities, and within joint international projects reveal growing interest in computational methods that not only interpret experimental data but also purposefully predict the properties of new compounds. The main focus of Tajik researchers is on three groups of materials, including kinetically stable kesterites, lead-free perovskites, as well as transition-metal oxides and oxynitrides used in photoelectric and catalytic systems.

Kesterite compounds based on Cu, Zn, Sn, Ge, and Se occupy a special place among the materials modeled by Tajik researchers using DFT. These semiconductors are characterized by elemental abundance, structural stability, and strong optical activity. Systems of the $Cu_2Ni(Sn,Ge,Si)Se_4$ and $Cu_2ZnSn(S,Se)_4$ type represent an important alternative to expensive and toxic compounds such as CdTe and CIGS that are traditionally used in solar cells [40, 41]. DFT modeling has shown that isoelectronic substitution S → Se leads to a smooth reduction of the band-gap width from approximately 1.6 eV to 1.1 eV and a shift of the absorption spectrum into the near-infrared region. This provides better matching with the solar spectrum and a potential increase in the absorption coefficient [42]. The use of SCAN and TB-mBJ functionals has made it possible to calculate optical constants and refractive indices with greater accuracy, demonstrating good agreement with

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experimental data. For modified $Cu_2Ni(Sn,Ge,Si)Se_4$ systems, band-structure calculations have confirmed that the introduction of Ge and Si increases the gap width and redistributes the density of states near the Fermi level. Such effects open the possibility of engineering control over semiconductor parameters in order to optimize photovoltaic efficiency. Analyses of the density of states show that the valence band is formed mainly by Cu and Se d orbitals, while the conduction band is formed by Sn or Ge s and p orbitals, which agrees with spectroscopic measurements [43, 44]. In addition to band characteristics, Tajik researchers pay attention to calculations of optical functions, including dielectric permittivity, reflectivity, and electron energy-loss function. These parameters make it possible to evaluate the interaction of light with the material, to determine transparency limits, and to characterize optical responses in different spectral ranges, which is crucial for the development of thin-film solar cells [45].

Lead-free perovskites based on tin, including $CsSnX_3$ with X equal to I, Br, or Cl, represent another actively studied group of compounds in Tajikistan. DFT modeling of these materials is aimed at identifying environmentally safe and thermally stable alternatives to classical Pb-containing perovskites [46].

Calculations have shown that halide-anion substitution leads to a systematic increase in the band-gap width, from approximately 1.3 eV for $CsSnI_3$ to approximately 2.6 eV for $CsSnCl_3$, as well as to changes in dielectric and optical properties. Optimization of crystal structure and phonon calculations have revealed the absence of imaginary modes in the spectrum, which indicates dynamic phase stability at room temperature [47]. Special attention has been paid to the study of phase transitions between tetragonal, orthorhombic, and cubic structures. Calculations show that during the transition to the cubic phase there is compression of energy levels and a shift in the Fermi level, which directly affects the material's conductivity and photosensitivity. Analyses of thermodynamic potentials have made it possible to establish temperature ranges in which perovskites remain stable and to determine the conditions under which transitions between phases occur [48]. Comparison of calculated and experimental values of the absorption coefficient has shown that a DFT model based on the SCAN and HSE06 functionals adequately describes the photoactivity of perovskites, especially in the 1.0–2.0 eV region characteristic of solar spectra.

An important direction of the Tajik DFT-modeling school is the analysis of oxides and oxynitrides that are used in photocatalytic systems and water-treatment devices. Of particular interest are TaON, $BaNbO_2N$, and ZrO_2, which possess a wide band gap and high chemical stability [50, 51].

Calculations have shown that substitution of Nb or Ta atoms with elements of lower valence, including Mg, V, or Al, can reduce the band-gap width, expand the absorption range, and increase photocatalytic activity in the visible region. Analyses of phonon spectra have confirmed the stability of doped structures, while calculated defect formation energies have shown that such substitutions are thermodynamically possible at moderate synthesis temperatures [52]. Separate attention has been paid to modeling water adsorption on oxide surfaces, in particular on ZrO_2 and Y-doped modifications. DFT calculations have made it possible to determine energetically preferred configurations of water molecules on the (101) and (001) surfaces, as well as to compute adsorption energies and diffusion barriers. The results show that the interaction of H_2O with the surface is accompanied by the formation of stable hydroxyl complexes, which is important for understanding catalytic processes and corrosion resistance [53, 54].

A characteristic feature of the Tajik scientific school is the pursuit of a comprehensive approach that combines DFT modeling with experimental investigations. In many cases, theoretical results, including structure, band gap, and frequency dependencies of reflectivity and absorption coefficients, are consistent with experimental data obtained by spectroscopy, X-ray diffraction, and thermography [55].

This agreement confirms the reliability of DFT predictions and opens up possibilities for their practical use in the design of new photocatalytic coatings, thermoelectric modules, and solar cells. Thus, Tajik scientists successfully integrate DFT modeling into national priorities for the

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development of renewable energy and nanotechnology, forming a foundation for subsequent industrial deployment.

4. Current Achievements and the Contribution of the DFT-Modeling School

The current stage of development of the Tajik school of theoretical materials science is characterized by the active introduction of quantum-mechanical modeling methods into interdisciplinary research, from the design of photoactive compounds to the analysis of energy-exchange mechanisms in oxide and perovskite structures. The application of DFT approaches has become an integral part of research programs aimed at developing new materials for renewable energy, hydrogen technologies, and optoelectronics. The main achievement of the Tajik research community is that DFT is no longer regarded merely as an auxiliary theoretical tool and has become a full component of the scientific cycle of modeling, synthesis, characterization, and optimization. Thanks to this approach, several significant results comparable to global trends have been achieved in recent years [4–21].

The development of DFT in Tajikistan is closely linked to the internationalization of research and the expansion of collaboration with leading foreign universities and centers. Joint projects with Japan, China, and the countries of the European Union have made it possible not only to improve computational infrastructure but also to strengthen the competencies of young specialists. Within partnerships with Japanese universities, methods of precision modeling of the optical properties of oxynitrides and perovskites are being actively mastered, which contributes to the formation of a stable research base in the field of photoenergy materials [56]. At the same time, collaboration with Chinese colleagues is focused on modeling photocatalytic water splitting, calculating surface states, and creating heterostructured systems based on TaON and $BaNbO_2N$. International grants and programs that support young scientists, including those of the CIS and Japan, have made it possible to expand computational capabilities and implement modern packages for high-precision DFT calculations. As a result, Tajik researchers have become active participants in the global scientific network, occupying a worthy place in the field of sustainable energy and advanced materials.

One of the most promising directions of the Tajik school is the integration of DFT with machine learning methods. This synergy opens up new horizons for property prediction and accelerated discovery of functional compounds. Based on large datasets obtained from DFT modeling, algorithms are created that can predict band-gap width, defect formation energy, carrier mobility, and absorption coefficients without the need for labor-intensive ab initio calculations. Such hybrid DFT–ML models already demonstrate high accuracy in tasks such as kesterite structure optimization, perovskite stability prediction, and selection of photocatalytic oxynitrides. This approach is especially relevant for countries with limited computational resources, since it substantially reduces calculation time while maintaining accuracy comparable to that of hybrid functionals. In addition, the use of machine learning in combination with DFT helps analyze correlations among structural, electronic, and optical characteristics, making it possible to identify hidden patterns and universal principles of materials design. In this way, the Tajik school demonstrates its ability not only to reproduce existing approaches but also to create its own algorithmic solutions aimed at automating scientific calculations [56, 57].

A characteristic feature of Tajik DFT studies is their interdisciplinary nature, where calculations are actively integrated with experimental methods of synthesis and diagnostics. The combination of quantum-chemical modeling with X-ray diffraction, electron microscopy, photoluminescence spectroscopy, and impedance spectroscopy makes it possible not only to confirm the reliability of theoretical predictions but also to clarify the nature of defect states and charge transport mechanisms [58].

In particular, calculated data on band-gap width, electronic densities of states, and absorption coefficients are successfully compared with experimental measurements carried out in the laboratories of the National Academy of Sciences of Tajikistan. Such an interplay of theory and experiment ensures a high level of reproducibility and turns DFT modeling into a real tool for

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predicting the properties of new materials, rather than a purely academic method. The introduction of DFT-based approaches also contributes to the training of a new generation of researchers who possess both computational and experimental skills, which is critical for the sustainable development of national science.

The application of DFT modeling in Tajik science helps address the challenges outlined in the strategies for the development of science and technology of the Republic of Tajikistan until 2030. Priority areas include renewable energy, nanomaterials, environmental protection, and the development of digital technologies. In these areas, DFT serves as a versatile instrument, from designing photoactive layers for solar cells to optimizing catalysts for hydrogen technologies and analyzing the stability of nanostructured coatings. The creation and development of a national DFT-modeling school has not only scientific but also socio-economic significance, since it contributes to the transition to a high-technology knowledge-based economy driven by scientific innovation. Thus, Tajik researchers make a tangible contribution to the development of fundamental and applied science in the region, combining the traditions of academic research with modern quantum-modeling methods.

5. Prospects and Directions for the Further Development of DFT Research

The development of DFT modeling in Tajikistan represents an important avenue of scientific and technological modernization. Current trends show that further progress in this field is associated with the expansion of computational resources, the introduction of hybrid DFT–ML approaches, the formation of national research consortia, and the strengthening of international scientific collaboration.

One of the main tasks for the coming years is the creation and development of national computational infrastructure for high-precision quantum-mechanical calculations. Despite the presence of individual local servers and university clusters, a large share of complex DFT projects is still carried out within international agreements and with the support of foreign partners. The creation of a centralized National Supercomputing Center would provide Tajik scientists with access to modern computational resources and would stimulate competitive research in materials science, solid-state physics, and nanotechnology. The experience of similar centers in Kazakhstan, Russia, and Uzbekistan shows that the presence of a powerful computational base accelerates scientific development and increases publication activity. In addition, infrastructure development may include the creation of a national database of DFT results, similar to the Materials Project or the NOMAD Repository, where the results of calculations by Tajik researchers would be accumulated. This would enable cross-validation of data, speed up the preparation of publications, and create a platform for interdisciplinary collaboration.

One of the most promising areas of further development is the introduction of artificial intelligence and automated workflows in the DFT-modeling process. The use of AI algorithms for preliminary selection of functionals, k-point meshes, and calculation parameters can significantly reduce modeling time without loss of accuracy. International experience shows that the combination of DFT and machine learning enables accelerated screening of thousands of potential compounds and prediction of their key properties, from band-gap width to thermodynamic stability [45]. For Tajikistan, the introduction of such tools is especially important, since it compensates for limited computational resources and increases the efficiency of scientific research. There are also plans to develop automated DFT platforms that allow students and young researchers to perform calculations without deep programming knowledge using visual interfaces. This will create a favorable environment for attracting a new wave of researchers to computational materials science and will raise the level of digital competence.

A key element of sustainable development is the formation of national research consortia that bring together universities, academic institutes, and research laboratories. Such structures can act as coordination centers for joint DFT projects and for organizing conferences and professional-development courses.

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The creation of specialized master's and doctoral programs in computational physics and quantum chemistry at Tajik universities will make it possible to train a new generation of specialists who possess DFT, ML, and experimental verification methods. Collaboration with foreign partners, in particular with universities in Japan, China, and Germany, is already laying the foundation for international educational programs, dual-degree tracks, and research internships [59]. In parallel, it is important to develop an internal system of scientific mentorship and to encourage the participation of young researchers in international competitions and grant programs. This will create a sustainable human-capital base and ensure the continuity of the Tajik school of quantum materials science.

An important direction for the future is the applied implementation of DFT-modeling results. The theoretical data obtained already make it possible to predict material behavior under real conditions, including the stability of photocatalysts under prolonged illumination, the degradation of perovskite layers under heating, and charge-transfer efficiency in kesterites. The establishment of close ties between academic institutions and industrial partners will open the way for the transfer of technologies based on DFT modeling. For example, computational data can be used to optimize synthesis parameters, select dopants, and predict device durability [60]. In the long term, such integration will make it possible to move from purely academic research to applied development, from modeling to prototypes and serial production.

The Tajik DFT-modeling school is already actively involved in the international scientific arena, yet further development requires closer participation in global open-data networks, conferences, and research initiatives. Participation in programs such as COST Actions, Horizon Europe, the BRICS STI Framework, and UNESCO Science Open Data will allow Tajik researchers not only to gain access to modern tools but also to contribute to international knowledge bases [61–66]. In addition, the creation of bilateral research platforms with Central Asian countries including Uzbekistan, Kazakhstan, and Kyrgyzstan will make it possible to form a regional center of competence in quantum materials science, combining resources and expertise to address shared challenges of sustainable development, energy security, and technological independence.

Summarizing the above, several key directions can be identified that define the future of DFT research in Tajikistan.

- Technological development involving the creation of national computational and information infrastructure.
- Scientific integration based on building stable collaborations and open databases.
- Educational transformation involving the incorporation of DFT methods into university curricula.
- An innovation-driven economy based on the transfer of computational technologies to the industrial sector.
- Global cooperation through active participation in international projects and scientific networks.

The implementation of these directions will enable Tajikistan not only to strengthen its position in computational science but also to turn DFT modeling into one of the key instruments of national technological independence.

Conclusion

The development of computational methods based on Density Functional Theory has opened new opportunities for scientific progress in Tajikistan, making it possible to move from descriptive analysis of material properties to their targeted design. In recent years, the country has formed a stable school of quantum-mechanical modeling focused on the study of functional compounds, including perovskites, kesterites, and transition-metal oxides and oxynitrides. These materials are key components of future technologies in photovoltaics, photocatalysis, thermoelectrics, and hydrogen energy.

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Tajik researchers have demonstrated that DFT methods can not only effectively describe the electronic structure and optical characteristics of materials but also serve as a tool for predicting their stability, defect structure, and thermodynamic behavior. As a result, the country has joined those who actively employ computational approaches to address the tasks of sustainable energy and materials science.

The achievements of the Tajik scientific school are based on a systemic approach that unites theoretical modeling, experimental verification, and international collaboration. This has led to significant results in quantum-chemical analysis of materials and has laid the foundation for training a new generation of specialists able to integrate DFT, machine learning, and nanotechnology methods into practical work.

Further development of DFT research in Tajikistan is associated with several key tasks, including the creation of national computational infrastructure and a database of DFT results, the development of educational and research programs in computational materials science, the introduction of hybrid approaches that combine quantum mechanics and artificial intelligence, the strengthening of international partnerships within Horizon Europe, BRICS, and the CIS, and the stimulation of applied research aimed at industrial use of computational data. The implementation of these directions will not only strengthen Tajikistan's position on the global scientific map but will also turn DFT modeling into a strategic instrument of sustainable development, technological independence, and the transition to a knowledge-based economy.

In the long term, the Tajik DFT school can become a hub for young scientists in Central Asia, capable of uniting regional efforts in quantum modeling, nanotechnology, and energy. In this way, the development of Density Functional Theory in the country becomes not only a scientific task but also an important element of state policy aimed at creating the intellectual and technological foundations of the future.

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