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# Adoption of Multi-Objective Grey Wolf Optimization (MOGWO) for Effective Analysis and Classification of Crystal Structures in Materials Science

**Imoh Ime Ekanem[1,*], Aniekan Essienubong Ikpe[2], Otobong Okon Ite[3]**

[1] Department of Mechanical Engineering, Akwa Ibom State Polytechnic, Ikot Osurua, Ikot Ekpene, Nigeria; imoh.ekanem@akwaibompoly.edu.ng.
[2] Department of Mechanical Engineering, Akwa Ibom State Polytechnic, Ikot Osurua, Ikot Ekpene, Nigeria; aniekan.ikpe@akwaibompoly.edu.ng.
[3] Department of Mechanical Engineering, University of Uyo, Nigeria; otobongite@gmail.com.

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## Abstract

In the field of materials science, the analysis and classification of crystal structures play a crucial role in understanding the properties and behaviour of materials. Traditional optimization algorithms have limitations in effectively handling the complex and multi-objective nature of this task. Therefore, there is a need for a more advanced and efficient optimization technique to address this challenge. This study focuses on the potential of adopting Multi-Objective Grey Wolf Optimization (MOGWO) for the effective analysis and classification of crystal structures in materials science. The methodology of this review involves a comprehensive analysis of existing literature on the application of MOGWO in materials science, particularly in the context of crystal structure analysis and classification. The review includes a critical evaluation of the strengths and limitations of MOGWO compared to traditional optimization algorithms. Additionally, classification, minimization, and optimization of crystal structures as well as structural stability, electrical properties, inter-atomic distance, lattice parameters, and phase transformation via MOGWO were also examined. The findings revealed that MOGWO offers several advantages over traditional optimization algorithms in the analysis and classification of crystal structures. For example, MOGWO is able to effectively handle the multi-objective nature of material crystal structures, providing more accurate and efficient results. Furthermore, MOGWO has been shown to outperform other optimization techniques in terms of convergence speed, improved accuracy, efficiency, and solution quality. The algorithm can effectively handle the complexity and multi-objective nature of problems in this field, providing more accurate results within the least possible time. This study highlights the potential of MOGWO as a valuable research tool in the field of materials science, offering a more efficient and effective approach that can advance our understanding of crystals.

**Keywords:** Grey wolf optimization, Crystal structures, Materials science, Inter-atomic distance.

## 1 | Introduction

Classification of crystal structures in materials science is a crucial aspect of understanding the properties and behaviour of materials. The arrangement of atoms in a crystal lattice determines many of the physical and

Corresponding Author: imoh.ekanem@akwaibompoly.edu.ng
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chemical properties of a material, such as its strength, conductivity, and optical properties. Various methods have been developed to classify crystal structures based on their symmetry, unit cell parameters, and atomic positions [1], [2]. In recent years, Multi-Objective Grey Wolf Optimization (MOGWO) has emerged as an effective tool for analyzing and classifying crystal structures. MOGWO is a metaheuristic optimization algorithm inspired by the hunting behaviour of grey wolves. It is based on the concept of dominance, where multiple objectives are optimized simultaneously to find a set of solutions that represent the trade-off between conflicting objectives. In the context of crystal structure classification, MOGWO can be used to optimize the parameters that define a crystal structure, such as lattice parameters, atomic positions, and symmetry operations [3–5].

By considering multiple objectives, MOGWO can provide a more comprehensive analysis of crystal structures compared to traditional optimization methods. The main objective of MOGWO is to find the optimal solution to a multi-objective optimization problem, where there are multiple conflicting objectives that need to be optimized simultaneously. In the case of crystal structure analysis, these objectives may include minimizing energy, maximizing stability, and optimizing other properties such as density or hardness [6], [7]. By considering multiple objectives at the same time, MOGWO is able to find a set of solutions that represent a trade-off between these conflicting objectives, known as the Pareto front. The concept of MOGWO is based on the principles of swarm intelligence, where a group of individuals works together to achieve a common goal. In this case, the grey wolves collaborate to explore the solution space and find the best possible solutions to the optimization problem [8]. The algorithm uses a combination of exploration and exploitation strategies, where the wolves search for new solutions in unexplored regions of the solution space while also refining existing solutions to improve their quality [9], [10]. One of the fundamental principles of MOGWO is the concept of dominance, where one solution is considered better than another if it is superior in at least one objective and not worse in any other objective. This principle is used to compare and evaluate the solutions found by the algorithm, allowing it to identify the Pareto front and select the best solutions for further analysis [11], [12]. MOGWO is a powerful algorithm for analyzing and classifying crystal structures in materials science. By considering multiple objectives simultaneously and using principles of swarm intelligence, MOGWO is able to find high-quality solutions that represent a trade-off between conflicting objectives. This algorithm has the potential to revolutionize the field of materials science by providing researchers with a powerful tool for optimizing and analyzing complex crystal structures.

## 2|Key Milestone in the Application of MOGWO to Crystal Structure Analysis

In recent years, MOGWO has emerged as a powerful tool for the analysis and classification of crystal structures, with the following key milestones:

I. Its ability to efficiently optimize multiple objectives simultaneously: traditional optimization techniques often focus on a single objective, which may not fully capture the complexity of crystal structures. MOGWO, on the other hand, is able to consider multiple objectives simultaneously, leading to more comprehensive and accurate analysis results [13], [14].

II. Its ability to handle large and complex datasets: crystal structures can be highly intricate and may contain a large number of atoms, making traditional analysis techniques computationally intensive and time-consuming. MOGWO's efficient optimization algorithm allows for the rapid analysis of large datasets, enabling researchers to quickly and accurately classify crystal structures [15], [16].

III. MOGWO has also been shown to be highly effective in identifying the most essential features of crystal structures. By optimizing multiple objectives, MOGWO is able to prioritize the most relevant characteristics of a crystal structure, leading to more meaningful and insightful analysis results. This can help researchers better understand the underlying factors that influence the properties of materials, leading to more informed decision-making in material design and development [17], [18].

Advancements in the field of material science have greatly benefited from the development of practical analysis and classification techniques for crystal structures. The ability to accurately characterize and classify crystal structures is crucial for understanding the properties and behaviour of materials, which in turn is essential for the design and development of new materials with specific desired properties [18]. The application of MOGWO to the analysis and classification of crystal structures represents a significant advancement in the field of material science. Its ability to optimize multiple objectives simultaneously, handle large datasets, and identify essential features of crystal structures makes it a valuable tool for researchers seeking to understand better and manipulate the properties of materials.

# 3 | Classification of Crystal via MOGWO

Crystal structures play a crucial role in the field of materials science, as they determine the physical and chemical properties of materials. In this study, the approach for classifying crystal structures in materials science using MOGWO is as follows:

I. The first step in the classification of crystal structures is to identify the lattice type and symmetry elements present in the structure. Lattice type refers to the arrangement of atoms in space, while symmetry elements are operations that leave the crystal structure unchanged. These elements include rotation, reflection, inversion, and translation. By identifying these elements, crystal structures can be classified into different space groups, which provide information about the symmetry and properties of the material [19], [20].

II. Once the lattice type and symmetry elements are identified, the next step is to analyze its properties using various techniques. One of the most effective methods for analyzing crystal structures is MOGWO optimization. MOGWO is a metaheuristic optimization algorithm inspired by the hunting behaviour of grey wolves. It is a powerful tool for solving multi-objective optimization problems, where multiple conflicting objectives need to be optimized simultaneously [21], [22].

III. After analyzing the properties of the crystal structures, the objectives of the optimization problem are defined. These objectives may include minimizing energy, maximizing stability, or optimizing other properties of the material [9].

IV. Once the objectives are defined, the next step is to select the crystal structures that will be considered in the optimization process. This step involves choosing a set of candidate structures that represent the different possible configurations of atoms in the material [23], [24].

V. After selecting the candidate structures, the next step is to define the constraints that must be satisfied during the optimization process. These constraints may include symmetry requirements, bond lengths, and other physical properties of the material. Once the objectives and constraints are defined, the MOGWO algorithm can be used to optimize the crystal structures [25], [26].

During the optimization process, the MOGWO algorithm iteratively updates the positions of the wolves in the search space based on their fitness values. The algorithm uses a set of parameters, such as the number of wolves, the convergence criteria, and the mutation rate, to control the search process. By iteratively updating the positions of the wolves, the algorithm converges to a set of Pareto-optimal solutions that represent the trade-offs between the different objectives of the optimization problem.

# 4 | Crystal Structure Optimization via MOGWO

In recent years, the use of optimization algorithms has become increasingly popular in the field of materials science, as they offer a systematic and efficient way to search for the optimal crystal structure. One such optimization algorithm that has shown promise in crystal structure optimization is the MOGWO algorithm. MOGWO is a metaheuristic algorithm inspired by the hunting behaviour of grey wolves, which allows for the simultaneous optimization of multiple objectives [27]. This makes MOGWO particularly well-suited for crystal structure optimization, as it can effectively balance competing objectives such as energy minimization, structural stability, and symmetry considerations. The procedure for crystal structure optimization via MOGWO typically involves the following stages:

I. Initialization: the optimization process begins with the generation of an initial population of candidate crystal structures. These structures are randomly generated or selected from a database of known crystal structures [28].

II. Fitness evaluation: each candidate's crystal structure is evaluated based on its fitness, which is typically determined by calculating the total energy of the structure using a suitable interatomic potential or density functional theory [29].

III. Grey wolf optimization: the MOGWO algorithm is applied to the population of candidate crystal structures to search for the optimal solutions. The algorithm iteratively updates the positions of the grey wolves (candidate solutions) based on their fitness and proximity to the alpha, beta, and delta wolves, which represent the best solutions found so far [30].

IV. Selection: after a certain number of iterations, the best crystal structures found by MOGWO are selected as the final optimized solutions Sharma [9]. These structures represent the most stable and energetically favorable arrangements of atoms within the crystal lattice.

V. Validation: the final optimized crystal structures are further validated using techniques such as molecular dynamics simulations or X-ray diffraction analysis to ensure their structural integrity and stability [31].

The use of MOGWO for crystal structure optimization in materials science offers a systematic and efficient approach to finding the most stable and energetically favorable arrangements of atoms within a crystal lattice. This can be achieved by the adoption of the aforementioned procedures for effective optimization of crystal structures in a wide range of materials and applications.

# 5 | Classifications of the GWO Algorithm for Crystal Structure Optimization

Various optimization algorithms have been developed to classify and optimize crystal structures in material science efficiently. One such algorithm is the Grey Wolf Optimizer algorithm, which is based on the hunting behaviour of grey wolves in nature, and classified as follows:

I. MOGWO is a metaheuristic algorithm that mimics the social hierarchy and hunting behaviour of grey wolves to optimize multiple objectives simultaneously. The algorithm consists of four main steps: initialization, fitness evaluation, ranking, and updating. In the initialization step, a population of grey wolves is randomly generated. In the fitness evaluation step, the fitness of each grey wolf is calculated based on the objective functions. The ranking step involves sorting the grey wolves based on their fitness values [32]. Finally, in the updating step, the grey wolves adjust their positions based on the alpha, beta, and delta values, which represent the best, second-best, and third-best solutions, respectively.

II. Another variant of MOGWO is the Multi-Objective Grey Wolf Optimizer with Dynamic Search Strategy (MOGWO-DSS). This variant incorporates a dynamic search strategy that adapts the search parameters based on the progress of the optimization process to improve the exploration and exploitation capabilities of the algorithm. The dynamic search strategy adapts the search parameters based on the convergence behaviour of the algorithm, allowing for a more efficient optimization process. By dynamically adjusting the exploration and exploitation rates, MOGWO-DSS effectively balances the trade-off between exploration of new regions and exploitation of promising solutions [33]. This adaptive strategy enables MOGWO-DSS to efficiently converge to high-quality solutions while maintaining diversity in the search space.

III. To further enhance the performance of the GWO algorithm for crystal structure optimization, there is also a novel variant known as the Multi-Objective Grey Wolf Optimizer with Opposite-Based Learning (MOGWO-OBL) [29]. This variant incorporates the concept of opposite-based learning, which aims to improve the exploration and exploitation capabilities of the algorithm by utilizing opposite solutions to guide the search process towards a more diverse and optimal solution space. The MOGWO-OBL algorithm is designed to simultaneously optimize multiple conflicting objectives in crystal structure

optimization problems, such as minimizing energy and maximizing stability [24]. The MOGWO-OBL algorithm has been shown to outperform traditional optimization algorithms in terms of convergence speed and solution quality for a wide range of crystal structure optimization problems. Its ability to effectively balance exploration and exploitation, along with its ability to handle multiple conflicting objectives, makes it a promising tool for materials scientists seeking to optimize crystal structures for various applications.

MOGWO and its variants offer a powerful and efficient approach to classifying and optimizing crystal structures in material science [34]. By simultaneously optimizing multiple objectives and incorporating dynamic search strategies, these algorithms can effectively explore the solution space and find optimal crystal structures for various applications.

# 6 | Minimization of Energy of Crystal Structures via MOGWO

Energy minimization is a crucial aspect in the field of materials science, particularly when it comes to studying crystal structures. This is aimed at finding the most stable configuration of atoms within a crystal lattice, which can provide valuable insights into the properties and behaviour of materials. In recent years, the use of optimization algorithms, such as MOGWO, has gained popularity in the field for its ability to minimize energy and optimize crystal structures [22] efficiently. The indication for minimizing energy in crystal structures lies in the fact that the stability and properties of materials are directly influenced by the arrangement of atoms within their crystal lattice. By so doing, the most energetically favorable configuration of atoms, which can help in predicting the mechanical, thermal, and electronic properties of materials, is identified. By optimizing crystal structures through energy minimization, the performance of materials in various applications, such as electronics, photonics, and catalysis, can be enhanced. Minimizing energy in crystal structures through MOGWO optimization is a valuable tool in materials science that can provide deep insights into the properties and behaviour of materials [35]. The use of MOGWO in energy minimization represents a significant advancement in the field, offering a powerful and efficient approach to exploring the vast landscape of materials design. Moreover, it aids the simultaneous optimization of multiple parameters in energy minimization problems.

# 7 | Optimization of Structural Stability in Crystal Structures via MOGWO

Structural stability plays a crucial role in determining the physical and chemical properties of materials in materials science. It refers to the ability of a crystal structure to maintain its integrity and resist deformation under external forces or changes in temperature and pressure. Optimizing structural stability is essential for enhancing the performance and reliability of materials in various applications [36], [37]. In recent years, MOGWO has emerged as a powerful tool for optimizing structural stability in crystal structures. Optimizing structural stability using MOGWO involves the simultaneous consideration of multiple objectives, such as minimizing energy, maximizing stability, and improving mechanical properties. By incorporating these objectives into the optimization process, MOGWO can effectively search for optimal solutions within the crystal lattice that balance different performance criteria [38]. The significance of optimizing structural stability using MOGWO lies in its ability to accelerate the discovery and development of advanced materials with enhanced properties. By efficiently exploring the design space and identifying optimal solutions, MOGWO can aid in overcoming the limitations of traditional trial-and-error approaches [39]. This can lead to the development of more efficient and sustainable materials that address pressing societal challenges, such as climate change, energy storage, and healthcare, while paving the way for new discoveries and applications in various industries.

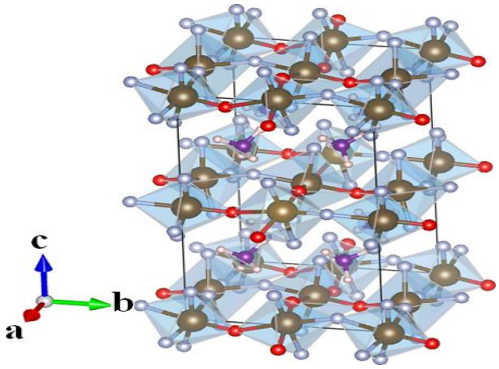


**Fig. 1. Structural stability in crystal structures [40].**

## 8 | Optimization of Electronic Properties in Crystal Structures via MOGWO

The optimization of electronic properties of crystal structures plays a crucial role in the design and development of advanced materials with tailored functionalities. Electronic properties such as band gap, conductivity, and dielectric constant are key factors that determine the performance of materials in various applications ranging from electronics to energy storage [41]. One promising approach for optimizing electronic properties of crystal structures is the MOGWO algorithm, which can effectively explore a vast design space and predict novel materials with desired properties. MOGWO is a nature-inspired optimization algorithm based on the hunting behaviour of grey wolves in nature. By mimicking the social hierarchy and hunting strategies of grey wolves, MOGWO has been shown to effectively optimize multiple conflicting objectives simultaneously, making it well-suited for the multi-objective optimization of electronic properties in materials science [42]. Optimizing electronic properties of crystal structures via MOGWO depends on its ability to efficiently search for materials with superior electronic properties compared to traditional trial-and-error methods. By simultaneously considering multiple objectives such as band gap, conductivity, and dielectric constant, MOGWO can identify optimal solutions that strike a balance between different properties, leading to the discovery of materials with enhanced performance [43]. This has the potential to accelerate the discovery of new materials with tailored electronic properties. By leveraging the computational power of MOGWO, it can efficiently explore a vast design space and identify promising candidates for further experimental validation. The impact of optimizing electronic properties of crystal structures via MOGWO extends beyond materials science to various fields such as electronics, photonics, and energy storage [44]. For example, materials with optimized band gaps can be used in solar cells to improve energy conversion efficiency, while materials with enhanced conductivity can be employed in electronic devices for faster data transmission.

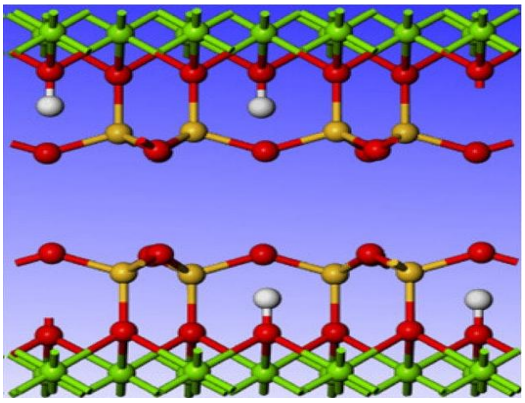

**Fig. 2. Electronic properties in crystal structures [45].**

## 9 | Optimization of Inter-Atomic Distance in Material Crystal Structures via MOGWO

Optimizing inter-atomic distances in crystal structures is a crucial aspect in materials science and engineering. This process involves adjusting the distances between atoms within a crystal lattice to achieve desired properties and performance characteristics [46]. MOGWO is a powerful computational technique that can be employed to optimize inter-atomic distances in crystal structures, leading to significant improvements in material properties [47]. The optimization process, which explores the molecular space within the structural lattice, is based on the fact that the arrangement of atoms within the lattice directly influences the physical and chemical properties of the material. By adjusting the distances between atoms, it is possible to enhance properties such as strength, conductivity, and thermal stability [48]. This optimization process can also lead to the achievement of optimal solutions that balance competing objectives, such as maximizing strength while minimizing weight or cost, as well as the development of new materials with unique properties that are not achievable through conventional methods. For example, optimizing inter-atomic distances in a semiconductor crystal structure can improve its electronic properties, leading to more efficient electronic devices [49]. Similarly, optimizing inter-atomic distances in a metal alloy can enhance its mechanical properties, making it more suitable for structural applications.

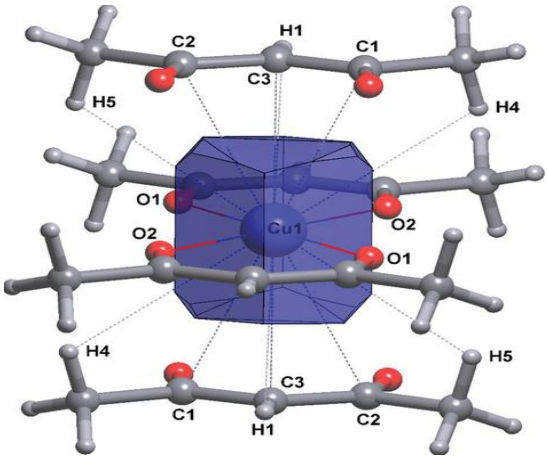


**Fig. 3. Inter-atomic distance in material crystal structures [50].**

# 10 | Optimization of Lattice Parameters in Material Crystal Structures via MOGWO

Optimizing lattice parameters of crystal structures is a crucial aspect in materials science that plays a significant role in determining the properties and performance of materials. Lattice parameters refer to the dimensions and angles of the unit cell in a crystal structure, which define the arrangement of atoms or ions within the crystal lattice.

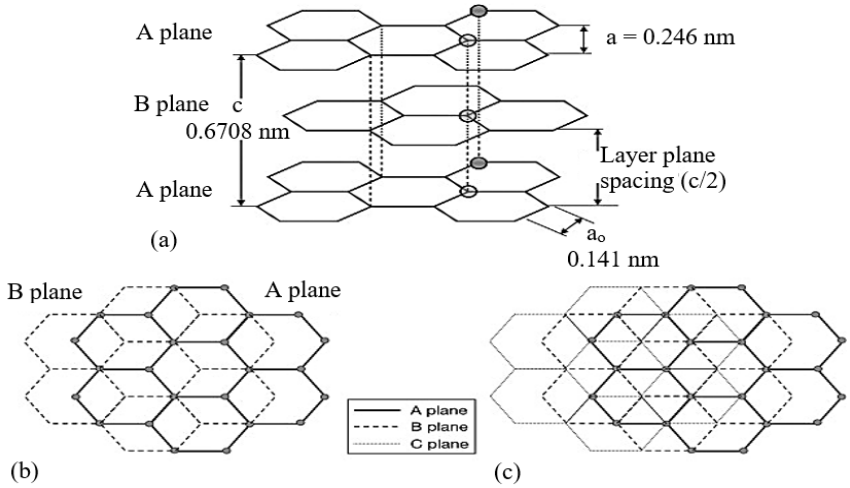


**Fig. 4. Lattice parameters in material crystal structures [51].**

MOGWO is an effective computational tool that can be employed in the optimization of lattice parameters to achieve the desired material properties and enhanced performance of materials in various applications [52]. This can aid in controlling the structural characteristics of materials such as bond lengths, bond angles, and interatomic distances. It can also allow for the customization of material properties such as mechanical strength, thermal conductivity, electrical conductivity, and optical properties to meet the requirements of different industries and technologies. The procedure for optimizing lattice parameters in material crystal structures via MOGWO involves the following key steps:

I. Problem formulation: define the objective functions and constraints for optimizing the lattice parameters in the material crystal structure. These objectives may include minimizing energy, maximizing stability, or optimizing mechanical properties [53].

II. Initialization: initialize a population of grey wolves representing potential solutions to the optimization problem. Each grey wolf is assigned a position in the search space corresponding to a set of lattice parameters [54].

III. Fitness evaluation: evaluate the fitness of each grey wolf in the population based on the objective functions and constraints defined in the problem formulation. This step determines the quality of each solution and guides the search process towards optimal solutions [55].

IV. Dominance ranking: rank the grey wolves in the population based on their fitness values using dominance ranking. This step helps identify the Pareto-optimal solutions that represent the best trade-offs between conflicting objectives [56].

V. Grey wolf optimization: apply the MOGWO algorithm to update the positions of grey wolves in the population. The algorithm uses the hunting behaviour of grey wolves to explore the search space and improve the quality of solutions over multiple generations [57].

VI. Convergence analysis: monitor the convergence of the optimization process by tracking the fitness values of the best solutions over time. This analysis helps determine when to stop the optimization process and select the final optimized lattice parameters [58].

VII. Solution selection: select the Pareto-optimal solutions from the final population of grey wolves as the optimized lattice parameters for the material crystal structure. These solutions represent the best trade-offs between the multiple objectives considered in the optimization process [59].

The significance of optimizing lattice parameters lies in the ability to solve complex optimization problems in material science, while improving the performance and functionality of materials. By fine-tuning the crystal structure through lattice parameter optimization, the stability, durability, and efficiency of materials in various environments and operating conditions can be enhanced.

## 11 | Prediction of Phase Transitions in Material Crystal Structures via MOGWO

Phase transitions in crystal structures play a crucial role in determining the physical and chemical properties of materials. Predicting these phase transitions accurately is essential for understanding the behaviour of materials under different conditions [60]. In recent times, MOGWO has emerged as a powerful tool for predicting phase transitions in crystal structures. The prediction of phase transitions in crystal structures refers to the process of determining the conditions under which a material transitions from one phase to another. This transition can involve changes in the arrangement of atoms, the symmetry of the crystal lattice, or the physical properties of the material [61]. The essence of predicting phase transitions using MOGWO includes the need for a robust optimization algorithm that can handle multiple objectives simultaneously. Additionally, MOGWO can handle non-linear and non-convex objective functions, making it ideal for predicting phase transitions in crystal structures. The procedure for predicting phase transitions in crystal structures using MOGWO involves several key stages. First, the objective functions and constraints for the optimization problem must be defined based on the specific phase transition of interest [19]. Next, the initial population of grey wolves is randomly generated, and the fitness of each individual is evaluated using the objective functions. The grey wolves then update their positions based on their hunting behaviour, with the alpha, beta, and delta wolves leading the search for optimal solutions. Finally, the algorithm converges to a set of Pareto-optimal solutions that represent the trade-offs between the competing objectives [62]. The significance of predicting phase transitions using MOGWO lies in its ability to provide accurate and reliable results in a timely manner. By exploring the potential of MOGWO, the phase space of materials can be effectively explored, and the conditions under which phase transitions occur can be identified.

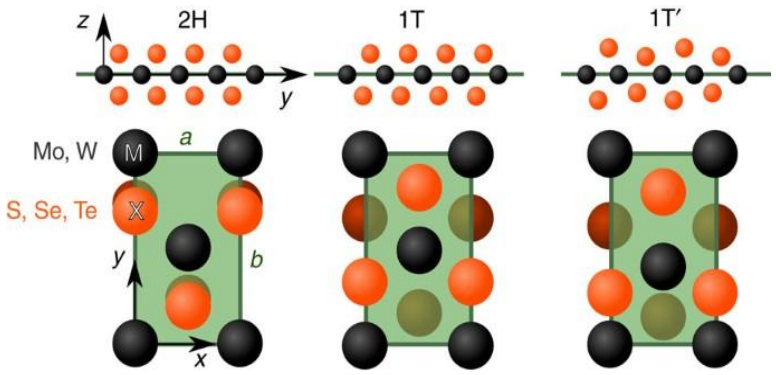


**Fig. 5. Phase transitions in material crystal structures [63].**

## 12 | Optimization of Symmetry Operations of Material Crystal Structures via MOGWO

Symmetry operations are essential for understanding the arrangement of atoms within a crystal lattice and can provide valuable insights into the physical and chemical properties of materials [48]. Symmetry operations

optimization involves the systematic exploration of the symmetry elements present in a crystal structure to identify the most efficient way to describe its symmetry. This process is fundamental in materials science, where the properties of a material are often directly related to its crystal structure [64]. By optimizing symmetry operations, hidden symmetries, structural defects or anomalies, and underlying structure-property relationships can be uncovered. MOGWO has been used in recent times for optimizing symmetry operations on crystal structures, which have been effective in predicting and controlling the physical and chemical properties of materials. This can lead to the development of new materials with enhanced performance characteristics, such as improved mechanical strength, thermal conductivity, or electrical conductivity [65]. By accurately characterizing the symmetry of crystal structures, the efficiency of computational simulations, crystallographic analyses, and materials design processes can be improved. This can lead to more accurate predictions of material properties, faster development of new materials, and a deeper understanding of the fundamental principles governing crystal symmetry. Additionally, optimizing symmetry operations can facilitate the comparison of different crystal structures, aiding in the identification of structural similarities and differences between materials [66]. The procedure for optimizing symmetry operations in structural lattice via MOGWO are as follows:

I. Identify the crystal structure of interest and determine the symmetry elements present in the lattice.

II. Define the objective functions for optimizing symmetry operations, such as maximizing the number of symmetry elements or minimizing the deviation from ideal symmetry.

III. Implement the MOGWO algorithm to search for the optimal set of symmetry operations that best describe the crystal structure [67].

IV. Evaluate the results of the optimization process and compare them to existing symmetry descriptions of the crystal structure.

V. Refine the symmetry operations based on the optimization results and assess the impact on the overall symmetry of the crystal lattice [67].

VI. Validate the optimized symmetry operations through experimental techniques, such as X-ray diffraction or electron microscopy, to confirm their accuracy and reliability [68].

By adopting advanced optimization techniques, such as MOGWO, the development of new materials with tailored properties and improved performance characteristics can be achieved, advancing the field of materials science and engineering.

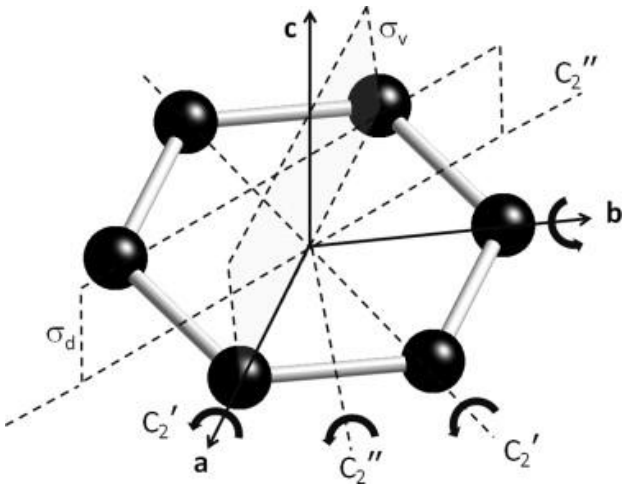


**Fig. 6. Symmetry operations of material crystal structures [69].**

# 13 | Factors that Influence the Implementation of MOGWO in the Classification of Crystal Structures

In recent times, MOGWO has emerged as a powerful tool for optimizing crystal structure classification in materials science. However, the implementation and performance of MOGWO in this context are influenced by the following factors:

I. The choice of objective functions plays a significant role in the implementation and performance of MOGWO for crystal structure classification. The objective functions should accurately capture the desired properties of the materials being studied and should be carefully selected to ensure that the optimization process converges to the desired solution [70].

II. The selection of parameters in the MOGWO algorithm can significantly impact its performance. Parameters such as the population size, the number of iterations, and the convergence criteria need to be carefully tuned to ensure that the algorithm converges to the optimal solution efficiently. Improper parameter selection can lead to premature convergence or slow convergence, which can hinder the performance of the algorithm [71].

III. The choice of encoding scheme also affects the implementation and performance of crystal structure classification via MOGWO. The encoding scheme determines how the crystal structures are represented in the optimization process and can significantly impact the search space and the efficiency of the algorithm. A well-designed encoding scheme can help the algorithm explore the search space effectively and converge to the optimal solution quickly [72].

IV. Furthermore, the quality of the initial population also plays a crucial role in the performance of MOGWO for crystal structure classification. A diverse and well-distributed initial population can help the algorithm explore the search space effectively and avoid getting stuck in local optima. Therefore, careful consideration should be given to the generation of the initial population to ensure that the algorithm performs optimally [73].

The implementation and performance of crystal structure classification in materials science via MOGWO are influenced by the aforementioned factors. By carefully considering these factors, the classification of crystal structures can be effectively optimized for improved material properties and behaviour.

# 14 | Conclusion

The adoption of MOGWO for the analysis and classification of crystal structures in materials science has shown promising results in this study. The use of the MOGWO algorithm has demonstrated its effectiveness

in optimizing multiple objectives simultaneously, leading to improved accuracy and efficiency in the analysis and classification of crystal structures. One of the key advantages of adopting MOGWO for this purpose is its ability to handle multiple conflicting objectives, such as maximizing accuracy while minimizing computational cost. This makes it a valuable tool in materials science, particularly in areas where optimization of analysis and classification processes is essential. Furthermore, the findings of this study have shown that MOGWO outperforms other optimization algorithms in terms of convergence speed and solution quality. Traditional optimization algorithms may struggle to effectively handle the multi-objective nature of these problems, leading to suboptimal solutions. MOGWO, on the other hand, has been shown to be highly effective in finding optimal solutions for multi-objective optimization problems in materials science. Its ability to handle multiple objectives and find optimal solutions makes it a promising algorithm for researchers looking to improve the efficiency and effectiveness of their crystal structure analysis and classification processes.

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