A Survey on Aflatoxin Remediation Using Modified Clays: Mechanisms and Applications

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Abstract

Aflatoxin contamination, primarily from Aspergillus species, poses severe health and economic challenges due to its potent carcinogenic properties, particularly aflatoxin B1 (AFB1). This survey paper explores the role of modified clays, such as montmorillonite, bentonite, and zeolite, in environmental remediation of aflatoxins. These clays exhibit unique adsorption mechanisms facilitated by their structural and chemical properties, enabling effective binding and removal of aflatoxins. The paper discusses various modification techniques—chemical, physical, and biological—that enhance clay adsorption capacities. Additionally, it highlights the integration of machine learning and computational models to optimize these processes. Practical applications, such as nanosulfur-bentonite composites and zeolite-containing oxide coatings, demonstrate the potential of these materials in real-world scenarios. Challenges in scaling and standardizing clay modifications are addressed, along with the need for innovative synthesis and characterization methods. The survey emphasizes the importance of integrating modified clays into broader remediation strategies to effectively manage aflatoxin contamination. Future research should focus on overcoming current limitations, enhancing technological advancements, and considering environmental and ecological impacts to develop sustainable solutions for safeguarding public health and environmental quality.

1 Introduction

1.1 Significance of Aflatoxin Contamination

Aflatoxin contamination presents a critical challenge to public health and economic stability, primarily due to the carcinogenic effects of aflatoxin B1 (AFB1) [1]. AFB1, a toxic metabolite produced by Aspergillus species, frequently contaminates food crops, leading to severe health risks, including liver cancer and other disorders [1]. The prevalence of aflatoxins is exacerbated by climate change and inadequate agricultural practices, increasing the risk of contamination and its health implications.

Economically, aflatoxin contamination undermines agricultural productivity, resulting in significant financial losses from reduced crop value and marketability [2]. The necessity for extensive remediation and control measures further burdens the agricultural sector, highlighting the urgent need for effective management strategies to mitigate these economic impacts [2]. Developing comprehensive detection and remediation technologies is essential to ensure food safety and quality.

The complex biosynthetic pathway of AFB1 involves numerous genes and enzymes, necessitating targeted interventions to control its production and prevent contamination [3]. Addressing the multifaceted challenges of aflatoxin contamination requires an integrated approach that enhances agricultural practices, advances detection and remediation technologies, and implements stringent regulatory frameworks to safeguard public health and food security [4].

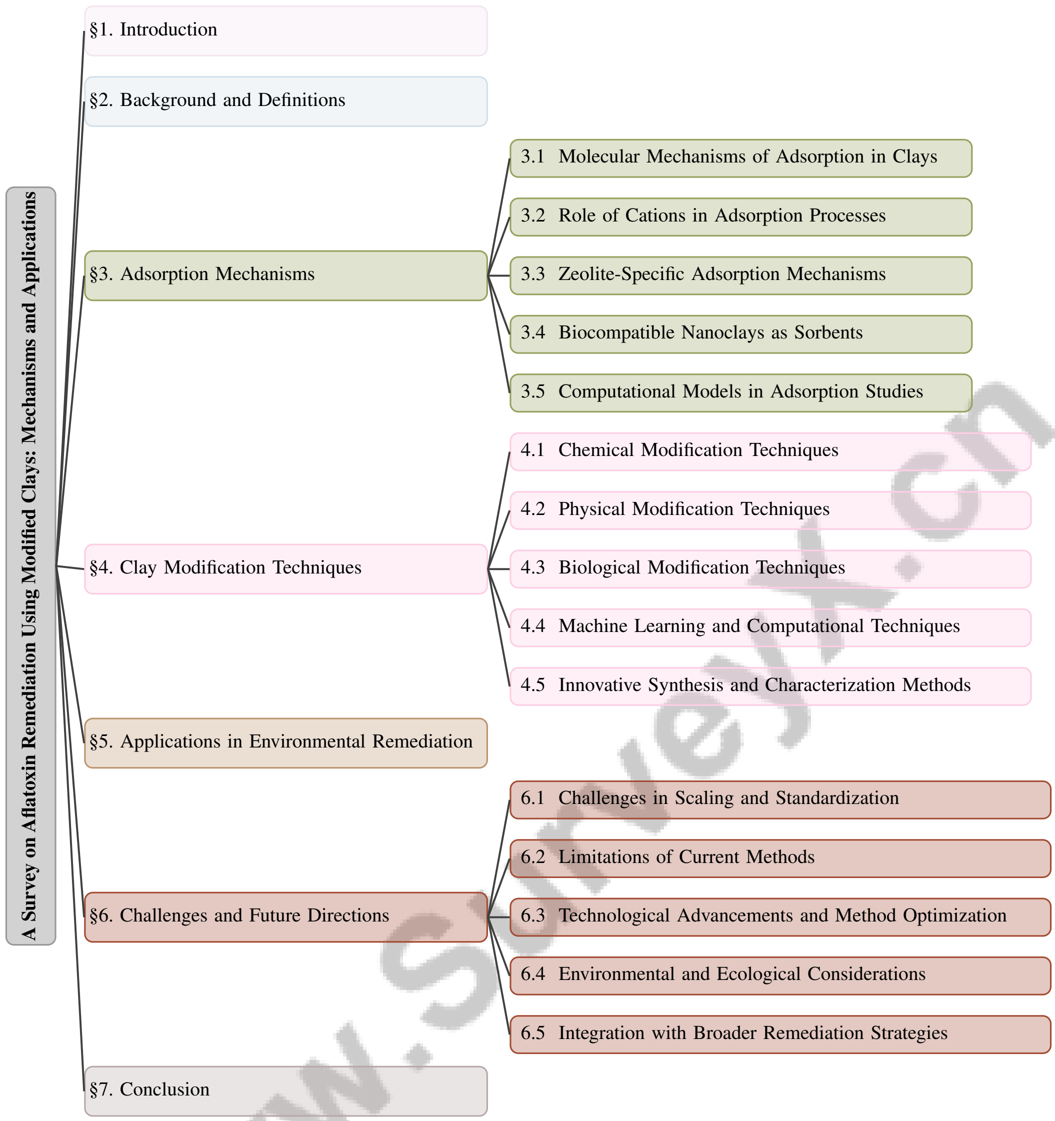

Figure 1: chapter structure

1.2 Role of Environmental Remediation

Environmental remediation plays a crucial role in addressing aflatoxin contamination, providing significant benefits such as improved food safety and reduced health risks [5]. The complexity of aflatoxin contamination necessitates a multifaceted approach that integrates detection, management, and remediation strategies to effectively mitigate its impact on human and animal health [6]. Despite advancements in detection and management, the lack of a universal method for aflatoxin reduction in food and feed remains a significant challenge, underscoring the need for innovative remediation technologies [2].

Modified nanoclays have shown promise in environmental applications due to their biocompatibility and effectiveness as sorbents for environmental contaminants [7]. Tailoring these materials can enhance their adsorption capabilities, providing a targeted approach to aflatoxin remediation. Current research has identified key genetic and regulatory mechanisms involved in aflatoxin biosynthesis, forming a foundation for developing targeted strategies to mitigate aflatoxin production in agricultural settings [3]. Leveraging these insights can optimize environmental remediation efforts to combat the global threat of aflatoxin contamination, ultimately enhancing food safety and reducing health risks [8]. Additionally, integrating computational chemistry into remediation strategies offers a deeper understanding of involved processes, fostering the development of more effective solutions [1].

1.3 Overview of Paper Structure

This survey is structured to provide a comprehensive understanding of aflatoxin remediation using modified clays, focusing on the mechanisms and applications of these materials. It begins with an introduction that emphasizes the significance of aflatoxin contamination and the essential role of environmental remediation in mitigating its adverse effects. The background section defines key terms and outlines the sources and impacts of aflatoxin contamination, as well as the properties and uses of clays like montmorillonite, bentonite, and zeolite in remediation efforts.

The survey primarily investigates the adsorption mechanisms that facilitate effective aflatoxin removal, highlighting the intricate molecular interactions involved and the significant role of cations in enhancing these processes. It examines how these mechanisms can be optimized to improve aflatoxin mitigation in food and feed, addressing health risks and economic impacts associated with contamination [9, 2, 6]. Specific attention is given to zeolite's unique adsorption mechanisms and the potential of biocompatible nanoclays as effective sorbents, alongside the application of computational models in predicting and optimizing these mechanisms.

Subsequent sections discuss various clay modification techniques, including chemical, physical, and biological methods, as well as innovative synthesis and characterization approaches. The integration of machine learning and computational techniques in optimizing these processes is also explored.

The paper further investigates practical applications of modified clays in environmental remediation, presenting case studies and examples of successful implementations. The concluding sections address challenges and future directions in scaling and standardizing clay modification processes, identifying current limitations, and exploring technological advancements and potential optimizations. Environmental and ecological considerations are discussed, along with strategies for integrating modified clays into broader remediation frameworks.The following sections are organized as shown in Figure 1.

2 Background and Definitions

2.1 Key Terms and Definitions

Aflatoxins are hazardous secondary metabolites predominantly produced by *Aspergillus flavus* and *Aspergillus parasiticus*, posing significant health risks via contaminated food and feed. Aflatoxin B1 (AFB1) is notably one of the most potent natural carcinogens, with its biosynthesis governed by intricate genetic and environmental factors. Effective detection and management are crucial, especially in regions with limited regulatory frameworks where impacts are most severe [8].

Montmorillonite, a natural clay mineral with a high cation exchange capacity, is effective in environmental remediation, particularly for adsorbing various contaminants, including aflatoxins [10]. Zeolites, with their microporous aluminosilicate structure, are significant in remediation due to their structural properties, such as pore size and chemical composition, which enhance adsorption capabilities [11, 4]. Their dielectric properties and relaxation mechanisms, especially in blends with polyaniline, highlight potential in advanced remediation technologies [12].

This survey classifies nanoclays, emphasizing their biocompatibility and efficacy in environmental remediation. It advocates for frameworks integrating systematic data acquisition and advanced model development to enhance the application of biocompatibly functionalized nanoclays in environmental challenges [13, 14, 7, 10, 15]. These frameworks are vital for advancing the use of modified clays in aflatoxin remediation.

2.2 Sources and Impacts of Aflatoxin Contamination

Aflatoxin contamination originates from *Aspergillus* species, particularly *Aspergillus flavus* and *Aspergillus parasiticus*, affecting crops like maize, peanuts, and tree nuts under high humidity and temperature. This complicates early detection and limits current management strategies [6]. Chronic dietary exposure to aflatoxins is linked to severe health risks, including liver cancer, highlighting its public health significance [2].

Beyond human health, aflatoxin contamination impacts animal health, causing reduced growth rates, immunosuppression, and increased disease susceptibility in livestock [9]. The genetic and environmental interactions in aflatoxin biosynthesis complicate prevention strategies, necessitating further research [3]. An interdisciplinary approach is essential, given healthcare data complexity and privacy concerns, underscoring the need for comprehensive detection methods and robust management strategies [16]. This highlights the importance of continued research and innovation [8].

2.3 Properties and Uses of Clays in Remediation

Montmorillonite, bentonite, and zeolite are pivotal in environmental remediation due to their distinctive adsorption properties essential for aflatoxin removal [15]. Montmorillonite, a smectite clay, is noted for its high cation exchange capacity and layered structure, enabling broad-spectrum contaminant adsorption, advantageous in aflatoxin remediation.

Bentonite, another smectite clay, is recognized for its swelling and absorption capabilities, which can be enhanced chemically to create effective superabsorbent polymer composites [17]. Its mechanical and swelling behaviors, optimized by ionic concentration adjustments, render it versatile for environmental applications, including aflatoxin adsorption [18].

Zeolites, with their microporous aluminosilicate framework, offer distinct remediation advantages due to high surface area and framework aluminum distribution, influencing adsorption capabilities [11]. Their unique porous structures are crucial for industrial applications [19]. Studies on 8-membered ring zeolites, like chabazite, reveal potential for catalytic and adsorption processes. Utilizing hydrated silicate ionic liquids (HSILs) as a growth medium has simplified zeolite synthesis, enhancing understanding of nucleation and structural properties [20].

Zeolite adsorption properties can be tailored through modifications, such as developing oxide coatings via plasma electrolytic oxidation, effective in photocatalytic degradation under visible light [21]. Zeolite RHO's pore deformations allow controlled adsorption, acting as a molecular valve [13]. Predicting zeolite adsorption properties remains challenging due to computational demands [22]. These innovations underscore zeolites' versatility and effectiveness in environmental remediation, particularly in contaminant adsorption, desorption, and recovery [23].

3 Adsorption Mechanisms

Understanding the interplay of adsorption mechanisms is pivotal in elucidating how aflatoxins interact with clay materials. This understanding is foundational for exploring the structural and chemical properties of clays like montmorillonite, bentonite, and zeolite, which facilitate effective adsorption processes. As illustrated in Figure 2, the hierarchical structure of adsorption mechanisms in clays encompasses various molecular mechanisms, including the role of cations, zeolite-specific mechanisms, biocompatible nanoclays, and computational models. Each of these categories is broken down into key properties, interactions, and applications, thereby offering insights into effective aflatoxin remediation strategies. The subsequent subsection delves into these molecular mechanisms, highlighting the complex interactions that make clays effective sorbents for aflatoxin remediation.

3.1 Molecular Mechanisms of Adsorption in Clays

The adsorption of aflatoxins onto clays such as montmorillonite, bentonite, and zeolite involves complex molecular interactions crucial for effective toxin binding and removal. These interactions are significantly influenced by the clays' surface area, cation exchange capacity, and structural characteristics [15]. Montmorillonite's high cation exchange capacity and layered structure support adsorption through wetting transitions, forming vesicles that encapsulate aflatoxins, thus enhancing removal [10]. The entropy-driven pumping mechanism further improves adsorption efficiency by leveraging the entropy of mixing [5].

Zeolites, with their microporous aluminosilicate framework, exhibit unique adsorption properties due to their crystalline structure. The interaction between cations and the negatively charged framework, mediated by water molecules, is crucial for hydration and effective aflatoxin adsorption [24]. Structural, energetic, and solvent effects on aflatoxin B1 (AFB1) influence the binding affinity and stability of aflatoxin-clay complexes [1].

Computational models, such as the EPCN model, enhance understanding by representing zeolite structures as graphs, where atoms are nodes and edges depict interactions [22]. This approach

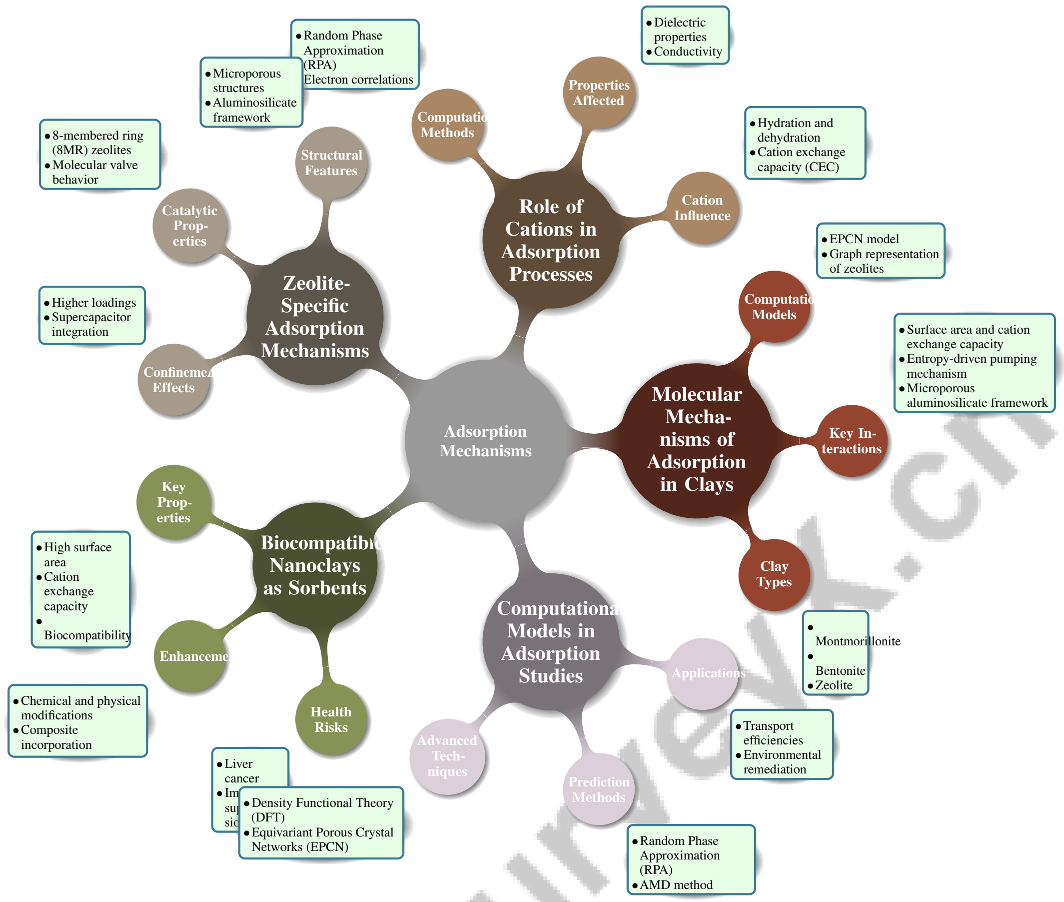

Figure 2: This figure illustrates the hierarchical structure of adsorption mechanisms in clays, highlighting molecular mechanisms, the role of cations, zeolite-specific mechanisms, biocompatible nanoclays, and computational models. Each category is broken down into key properties, interactions, and applications, offering insights into effective aflatoxin remediation strategies.

facilitates rapid prediction of adsorption properties, optimizing clay modifications for improved aflatoxin remediation.

Recent research has significantly advanced our understanding of aflatoxin contamination and remediation processes, leading to more effective control measures. Studies have highlighted health risks like liver cancer and oxidative stress, explored advanced detection techniques, and incorporated resistant crop varieties in animal feed. Innovations in biocompatible nanoclay functionalization have opened new avenues for environmental cleanup, demonstrating potential for improved remediation [7, 10, 2].

As illustrated in Figure 3, the hierarchical structure of molecular mechanisms involved in the adsorption of aflatoxins onto clays is highlighted, showcasing key concepts and interactions within montmorillonite, zeolites, and aflatoxin remediation strategies. The images included in this figure provide a comprehensive view of the intricate molecular interactions and structural dynamics that underpin these adsorption processes [25, 18, 10].

3.2 Role of Cations in Adsorption Processes

Cations are pivotal in enhancing the adsorption processes of clays like montmorillonite, bentonite, and zeolite by influencing their structural and chemical properties. In zeolites, cations significantly affect hydration and dehydration processes, as in clinoptilolite, where water adsorption is mediated through single molecule addition to cation sites [24]. This interaction is crucial for adsorption efficiency and stability.

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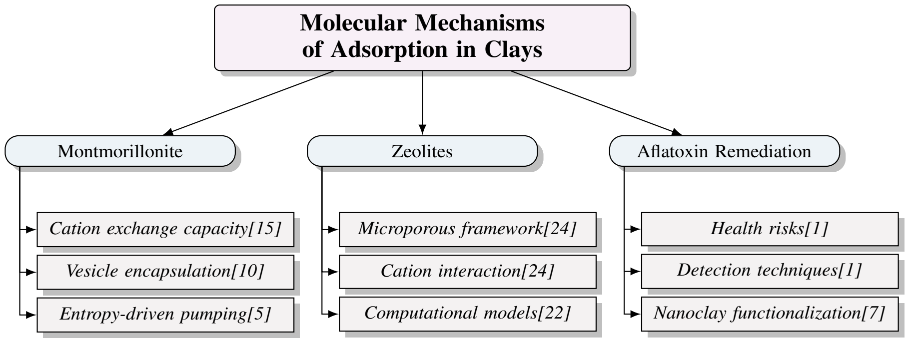

Figure 3: This figure illustrates the hierarchical structure of molecular mechanisms involved in the adsorption of aflatoxins onto clays, highlighting the key concepts and interactions within montmorillonite, zeolites, and aflatoxin remediation strategies.

The cation exchange capacity (CEC) of clays enhances their adsorption capabilities. Modifying zeolites to improve CEC facilitates more effective contaminant adsorption through ion exchange processes [23]. Cations also influence the dielectric properties and conductivity of clay composites, crucial for maintaining structural integrity and functionality [12].

Cations affect liquid structure and conductivity, vital for understanding zeolite nucleation and growth [20]. Computational methods like the Random Phase Approximation (RPA) with singles corrections accurately capture long-range electron correlations, aiding in understanding cation roles in molecular interactions [25, 14, 22]. These insights help design more effective clay-based adsorbents for environmental remediation.

3.3 Zeolite-Specific Adsorption Mechanisms

Zeolites, with their unique microporous structures, offer distinct adsorption mechanisms effective in aflatoxin remediation. Their aluminosilicate framework allows for selective adsorption of various molecules, including toxins. The Zeolite Sorting Hat tool, with 95

8-membered ring (8MR) zeolites are effective in catalysis and environmental remediation [26]. Their catalytic properties facilitate breakdown and adsorption of complex compounds. The structural flexibility of zeolites, influenced by extra-framework cation polarizing power, enhances molecular valve behavior and adsorption capacity [13].

Confinement effects within zeolite pores impact adsorption dynamics. Studies on silicalite-1 show confinement can lead to higher loadings than Langmuir model predictions [27]. Integrating zeolite frameworks in supercapacitor electrodes enhances charge retention, showcasing zeolite versatility beyond traditional adsorption [28].

3.4 Biocompatible Nanoclays as Sorbents

Biocompatible nanoclays are potent sorbents for aflatoxin remediation due to their structural and chemical properties. Their high surface area and cation exchange capacity are crucial for effective binding [7]. Biocompatibility ensures safety in environments with human and animal exposure, vital in agriculture where food safety is paramount. Chemical and physical modifications enhance adsorption capabilities, effectively targeting aflatoxins—highly toxic mycotoxins posing serious health risks like liver cancer and immune suppression [8, 2, 6, 9, 7].

Incorporating nanoclays into composites enhances sorption efficiency, especially when biocompatibly functionalized [7, 10, 29, 14]. Computational models aid in predicting and optimizing nanoclay sorption properties, facilitating effective remediation strategies.

3.5 Computational Models in Adsorption Studies

Computational models are crucial in elucidating and predicting aflatoxin adsorption mechanisms on clays like zeolites, montmorillonite, and bentonite. Advanced techniques like Density Functional

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Theory (DFT) study and predict zeolite adsorption properties, providing insights into governing interactions [11].

The Equivariant Porous Crystal Networks (EPCN) model, using machine learning, efficiently simulates complex interactions within porous structures [22]. The Random Phase Approximation (RPA) with singles corrections offers high-quality adsorption energies, outperforming the MP2 method [25].

As illustrated in Figure 4, the hierarchical structure of these computational models is categorized into DFT and RPA methods, machine learning models, and entropy-driven models. Each category highlights key techniques and their applications in understanding and predicting adsorption mechanisms for materials such as zeolites. The AMD method predicts inorganic synthesis conditions by calculating distances between zeolite structures, capturing structural similarities and differences [30]. Entropy-driven models enhance understanding of transport efficiencies in adsorption processes, guiding more effective aflatoxin remediation mechanisms [5].

These computational models provide a robust framework for studying and predicting clay adsorption mechanisms, facilitating innovative aflatoxin remediation solutions. Integrating advanced computational models with experimental data enhances understanding of environmental remediation techniques, improving our ability to tackle complex environmental contamination challenges [14, 2, 25, 7, 10].

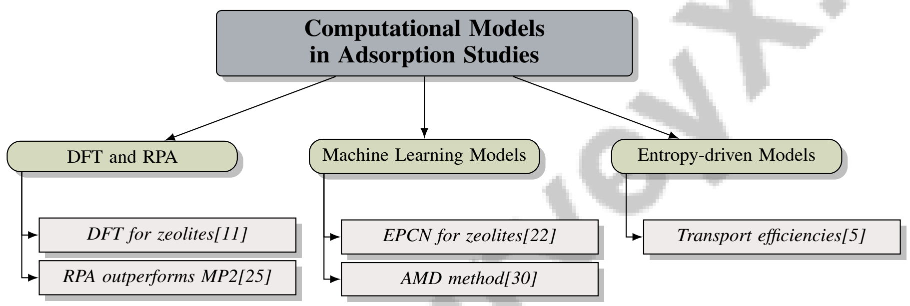


Figure 4: This figure illustrates the hierarchical structure of computational models used in adsorption studies, categorized into DFT and RPA methods, machine learning models, and entropy-driven models. Each category highlights key techniques and their applications in understanding and predicting adsorption mechanisms for materials such as zeolites.

4 Clay Modification Techniques

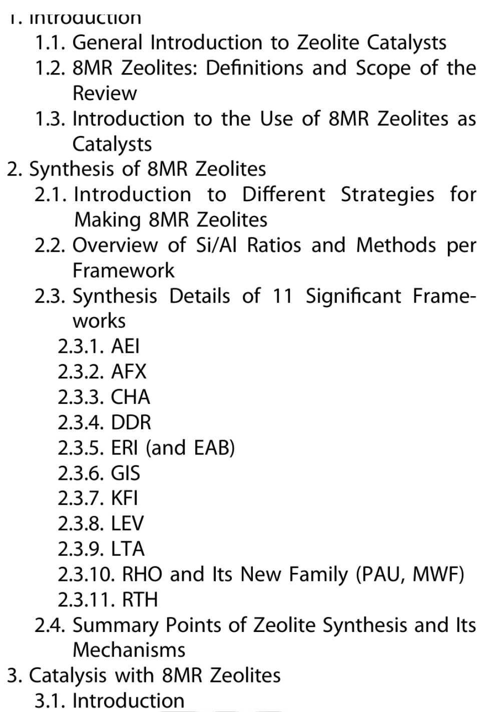
Category	Feature	Method
Chemical Modification Techniques	Adsorption Enhancement	DPM[12]
Biological Modification Techniques	Biological Enhancement	ZSH[14], EDP[5], ZTA[23]
Machine Learning and Computational Techniques	Molecular Simulation Techniques Graph and Distance Analysis	MD[20] AMD[30], EPCN[22]
Innovative Synthesis and Characterization Methods	Model Improvement Techniques Material Enhancement Methods	NNP[31] ZC-SC[28]

Table 1: Summary of various modification techniques and methods applied to enhance clay materials for environmental remediation. The table categorizes techniques into chemical, biological, machine learning and computational, and innovative synthesis and characterization methods, providing specific features and corresponding methods with relevant citations.

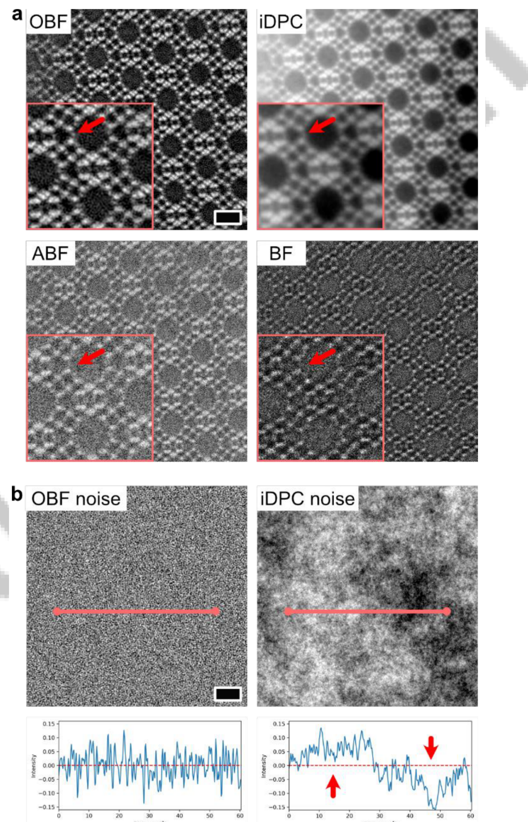
Various clay modification techniques have been developed to enhance the properties of clays for specific applications, particularly in environmental remediation. Table 1 presents a comprehensive overview of the diverse modification techniques utilized to enhance the properties of clay materials, particularly for applications in environmental remediation. Table 2 offers a detailed comparison of different clay modification techniques, showcasing their respective features and applications in enhancing clay properties for environmental remediation. This section explores diverse approaches, starting with chemical modification techniques that improve the adsorption capabilities of clays such as montmorillonite, bentonite, and zeolite. These techniques alter the surface chemistry of the clays, significantly influencing their interactions with contaminants and enhancing their efficacy in applications like aflatoxin remediation.

4.1 Chemical Modification Techniques

Chemical modifications are vital for enhancing clay adsorption properties, thereby improving their efficacy in aflatoxin remediation. Synthesizing nanosulfur-bentonite composites via sodium thiosulfate and sulfuric acid reactions significantly boosts adsorption capacity [29]. In zeolites, acid and alkaline treatments enhance ammonium ion adsorption by increasing cation exchange capacity [23]. Dielectric Permittivity Measurement (DPM) studies of zeolite-polyaniline blends provide insights into optimizing adsorption properties [12]. Furthermore, mechanical processes forming semi-permeable montmorillonite vesicles enhance adsorption while preserving natural properties [10]. These chemical modification techniques underscore the importance of surface modifications for improving aflatoxin remediation [9, 15].


1. Introduction
   1.1. General Introduction to Zeolite Catalysts
   1.2. 8MR Zeolites: Definitions and Scope of the Review
   1.3. Introduction to the Use of 8MR Zeolites as Catalysts
2. Synthesis of 8MR Zeolites
   2.1. Introduction to Different Strategies for Making 8MR Zeolites
   2.2. Overview of Si/Al Ratios and Methods per Framework
   2.3. Synthesis Details of 11 Significant Frameworks
      2.3.1. AEI
      2.3.2. AFX
      2.3.3. CHA
      2.3.4. DDR
      2.3.5. ERI (and EAB)
      2.3.6. GIS
      2.3.7. KFI
      2.3.8. LEV
      2.3.9. LTA
      2.3.10. RHO and Its New Family (PAU, MWF)
      2.3.11. RTH
   2.4. Summary Points of Zeolite Synthesis and Its Mechanisms
3. Catalysis with 8MR Zeolites
   3.1. Introduction

(a) Introduction to the Use of 8MR Zeolites as Catalysts[26]



(b) Comparison of Different Imaging Techniques in Electron Microscopy[19]

Figure 5: Examples of Chemical Modification Techniques

As shown in Figure 5, chemical modification techniques are pivotal, enhancing material properties through structured overviews of 8MR zeolites in catalysis and advanced imaging techniques in electron microscopy, highlighting the significance of these modifications in materials science [26, 19].

4.2 Physical Modification Techniques

Physical modification techniques enhance clay adsorption properties by altering their structure and increasing surface area and porosity. Mechanical processes, such as shear forces in montmorillonite suspensions, create semi-permeable vesicles for size-selective permeability [10, 18]. Bentonite's mechanical compression affects swelling behavior and absorption capacity, enhancing adsorption properties [18]. Thermal treatments modify zeolite structures, improving pore size and surface area for aflatoxin adsorption [26, 2]. Blending clays with polymers enhances adsorption and mechanical strength [8, 2].

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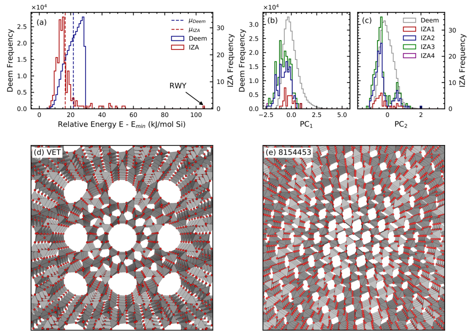
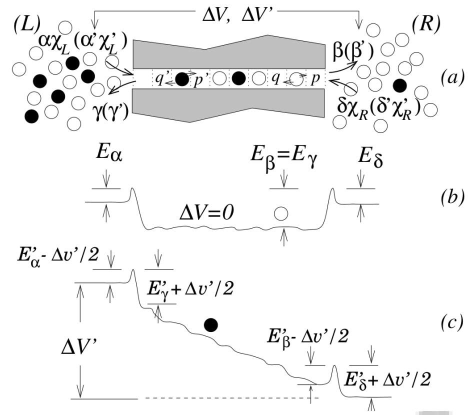


(a) Deem and IZA Frequency Distributions and Corresponding Structures[14]



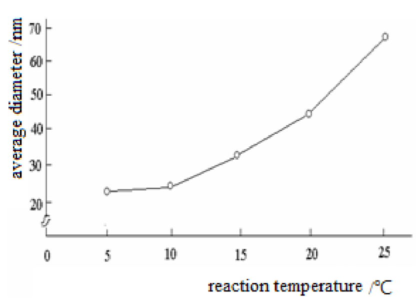
(b) The image depicts a schematic representation of a molecular system undergoing a phase transition.[5]

Figure 6: Examples of Physical Modification Techniques

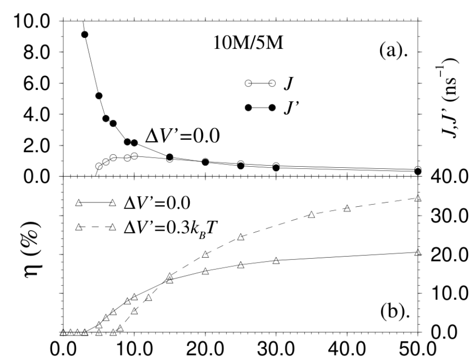
As shown in Figure 6, physical modification methods alter structural and surface properties without changing clay chemical composition. The first image compares Deem and IZA frequency distributions, while the second depicts a molecular phase transition, illustrating physical modifications' dynamic nature [14, 5].

4.3 Biological Modification Techniques

Biological modification techniques enhance clay adsorption capabilities using biological processes, creating biocompatible nanoclays with increased efficacy in environmental remediation [7, 10]. Microbial processes alter clay surface chemistry, enhancing adsorption through extracellular enzymes and metabolites [23]. Bio-based materials, like biopolymers, enhance adsorption due to synergistic effects with clay matrices [7]. Plant extracts introduce functional groups on clay surfaces, increasing contaminant affinity and aligning with green chemistry principles [7]. Biological modifications offer sustainable solutions for environmental challenges, necessitating ongoing research for large-scale applications [14].



(a) The graph shows the relationship between reaction temperature and the average diameter of a material.[29]



(b) The image shows a graph comparing the transient current density (J) and its derivative (J') for two different temperatures (V' = 0.0 and V' = $0.3k_BT)ina10M/5Melectrolytesolution.$[5]

Figure 7: Examples of Biological Modification Techniques

As shown in Figure 7, biological modification methods are highlighted through a graph showing the relationship between reaction temperature and average diameter in nanosulfur-bentonite complexes, and a graph comparing transient current density in an electrolyte solution. These examples illustrate temperature-material property relationships and electrical characteristics in modified clay systems [29, 5].

4.4 Machine Learning and Computational Techniques

Machine learning and computational techniques optimize clay modification processes, enhancing adsorption properties for environmental remediation. These methods model and predict clay performance, such as montmorillonite, bentonite, and zeolite, in aflatoxin remediation [10, 14]. The Equivariant Porous Crystal Networks (EPCN) model improves prediction accuracy of adsorption properties [22]. Density functional theory (DFT) modeling reveals zeolite structural and electronic properties, facilitating accurate simulations [31]. The Zeolite Sorting Hat classifies zeolite structures for remediation applications [30]. Molecular dynamics simulations of hydrated silicate ionic liquids (HSILs) enhance understanding of interactions in clay systems [20]. These techniques enable efficient identification of promising materials and synthesis conditions, improving environmental cleanup strategies [30].

4.5 Innovative Synthesis and Characterization Methods

Innovative synthesis and characterization methods enhance modified clays' efficacy in environmental remediation, particularly for aflatoxin adsorption. Advanced materials like modified clays adsorb toxic aflatoxins produced by *Aspergillus* species [2]. Large-scale simulations of siliceous zeolites capture structural diversity and phase transitions [31]. The Random Phase Approximation (RPA) with singles corrections offers accurate adsorption energy predictions [25]. Zeolite coatings on supercapacitor electrodes enhance stability and efficiency, improving clay modification processes [28]. These methods advance modified clays for aflatoxin remediation, promoting sustainability in environmental management [7].

Feature	Chemical Modification Techniques	Physical Modification Techniques	Biological Modification Techniques
Modification Type	Chemical Reactions	Structural Alteration	Biological Processes
Enhanced Property	Adsorption Capacity	Surface Area	Biocompatibility
Application Focus	Aflatoxin Remediation	Aflatoxin Adsorption	Environmental Remediation

Table 2: This table provides a comparative analysis of various clay modification techniques, categorized into chemical, physical, and biological methods. It highlights the type of modification, the enhanced properties achieved, and the primary application focus for each technique, particularly in the context of aflatoxin and environmental remediation.

5 Applications in Environmental Remediation

5.1 Nanosulfur-Bentonite Composites in Antifungal Treatments

Nanosulfur-bentonite composites are recognized for their potent antifungal properties and enhanced adsorption capacity. Synthesized through the reaction of sodium thiosulfate with sulfuric acid, these composites integrate nanosulfur into bentonite, which augments its cation exchange capacity and swelling behavior, thereby enhancing its function as a sorbent for environmental contaminants [29, 10]. Empirical evidence demonstrates their efficacy in reducing aflatoxin levels in contaminated materials, addressing fungal contamination while supporting environmental remediation objectives [15].

5.2 Zeolite Chabazite and Adsorption Energies

Zeolite chabazite, noted for its crystalline structure and high adsorption capacity, is pivotal in environmental remediation. Its adsorption efficiency is driven by the framework aluminum distribution and microporosity, facilitating selective contaminant adsorption [11]. The adsorption process is influenced by interactions between adsorbate molecules and the zeolite framework, modulated by extra-framework cations, which alter electrostatic potentials and adsorption strength [25]. Advanced computational methods like the Random Phase Approximation (RPA) accurately determine adsorption energies, providing insights into thermodynamics and enabling the design of chabazite with tailored properties for specific environmental applications [25]. Table 3 provides a detailed overview of the

Benchmark	Size	Domain	Task Format	Metric
ZP-PEO[21]	1,000	Photocatalysis	Photocatalytic Activity Evaluation	Photocatalytic degradation efficiency, Corrosion resistance

Table 3: This table presents a comprehensive overview of the ZP-PEO benchmark, which is utilized in the domain of photocatalysis. It details the benchmark size, domain, task format, and the metrics used for evaluating photocatalytic activity, including degradation efficiency and corrosion resistance.

ZP-PEO benchmark, highlighting its relevance in evaluating photocatalytic activity within the domain of photocatalysis.

5.3 Zeolite-Containing Oxide Coatings in Wastewater Treatment

Zeolite-containing oxide coatings significantly enhance photocatalytic activity and corrosion resistance in wastewater treatment. When immobilized on aluminum supports, these coatings improve contaminant degradation under visible light [21]. Zeolite's microporous framework and cation exchange capacity boost the photocatalytic efficiency, facilitating pollutant adsorption and degradation. The immobilization process via plasma electrolytic oxidation enhances mechanical stability and corrosion resistance, extending the treatment system's lifespan, especially with Ce-exchanged zeolites exhibiting superior photocatalytic activity. Processing conditions like pulsed DC regimes further optimize these properties, making modified aluminum supports effective for environmental remediation [7, 14, 21]. Integrating zeolite into oxide coatings improves pollutant degradation and serves as a corrosion barrier, enhancing wastewater treatment efficiency and sustainability [19, 26, 21].

5.4 Bentonite-g-poly(acrylate-co-acrylamide) Composites

Bentonite-g-poly(acrylate-co-acrylamide) composites are valued for their high water absorptivity and adsorption capabilities. Grafting poly(acrylate-co-acrylamide) onto bentonite enhances its swelling and absorption properties, creating a superabsorbent polymer composite ideal for moisture management [17]. The polymer chains' functional groups promote pollutant adsorption, improving environmental remediation efficiency, as demonstrated in studies on biocompatible nanoclays [7, 25, 10, 14]. The composite's high cation exchange capacity enhances its ability to adsorb heavy metals and ionic pollutants, making it suitable for various remediation scenarios. These composites are versatile in soil and water treatment, mitigating pollution and improving natural resource quality. Biocompatibly functionalized nanoclays effectively absorb and immobilize contaminants, preventing groundwater leaching and reducing toxin bioavailability in soil, significantly contributing to environmental remediation [5, 18, 2, 7, 10].

6 Challenges and Future Directions

6.1 Challenges in Scaling and Standardization

Scaling and standardizing clay modification processes for industrial applications present significant challenges, particularly in maintaining the quality and performance of nanosulfur-bentonite composites. The complexity of synthesis processes often leads to variability in production batches [9]. Effective aflatoxin control is hindered by the intricate biosynthetic pathways and environmental interactions, with many genes in the aflatoxin biosynthetic pathway remaining poorly understood [3]. Current treatment methods also struggle with varying environmental conditions [9].

Zeolites' potential cytotoxicity complicates standardization in environmental remediation, necessitating careful control of drug release profiles and biological interactions [4]. The absence of standardized data and insufficient model validation further impede the practical application of laboratory findings. Challenges in proposing inorganic conditions for new zeolite frameworks and limited field trials exacerbate these issues, particularly given the health risks associated with aflatoxin contamination, such as liver cancer and immune suppression [8, 2, 3, 6, 9].

Bentonite-based composites face scalability challenges due to complex mechanical properties, chemical interactions, and environmental responsiveness. Recent studies highlight the need for a deeper understanding of multi-field coupling mechanisms governing composite behavior, emphasizing the importance of developing standardized protocols and robust validation frameworks to bridge the gap between research and practical implementation [18, 10, 29, 17].

6.2 Limitations of Current Methods

Current clay modification methods for aflatoxin remediation face limitations affecting scalability and effectiveness in diverse environments [15]. Environmental variability complicates aflatoxin detection, particularly in resource-limited settings, necessitating more adaptable detection and remediation strategies [8]. Complex interactions involving aflatoxin B1 (AFB1) challenge the understanding of adsorption mechanisms on clays, as existing methods may not capture these complexities [1]. Methodologies also struggle with highly defective zeolites or extreme conditions, limiting applicability [13].

In zeolite applications, alkaline treatment can diminish adsorption capacity, indicating a need for further optimization for large-scale applications [23]. Direct imaging techniques require refinement to accommodate diverse zeolite types or materials with unique structures [19]. The limitations in current methods underscore the need for ongoing research to address the challenges posed by aflatoxin contamination, primarily caused by Aspergillus species, which pose severe health risks and impact agricultural economics. Advancing the understanding of clay's role in aflatoxin mitigation and developing innovative application techniques is crucial for enhancing food safety and public health [8, 2, 3, 6, 9].

6.3 Technological Advancements and Method Optimization

Advancements in clay modification methods are vital for enhancing adsorption efficacy, particularly in aflatoxin remediation. Research highlights the need to optimize synthesis processes for nanosulfur-bentonite composites and explore alternative carriers for antifungal applications [29]. Novel synthesis techniques and optimization for small-pore zeolites could improve adsorption processes [26].

Integrating machine learning and computational techniques, such as the Neural Network Potential (NNP) method, holds promise for optimizing clay modifications by achieving Density Functional Theory (DFT)-level accuracy at reduced costs, facilitating large-scale simulations and new zeolite framework discovery [31]. Refining the Zeolite Sorting Hat model and exploring additional structural features could enhance classification performance [14]. Future research should elucidate uncharacterized genes and environmental interactions to develop sustainable strategies for aflatoxin control [3]. Integrating computational and experimental approaches is recommended to optimize understanding of AFB1 mechanisms and develop effective remediation strategies [1].

Photocatalytic applications could benefit from optimizing cerium concentration and exploring other zeolite types to enhance photocatalytic coatings [21]. Incorporating adsorbate interactions could improve model applicability to other zeolite-adsorbate systems [27]. Biocompatible nanoclays, developed using environmentally friendly surfactants, represent an area of interest for real-world environmental remediation [7]. Optimizing microwave-assisted methods and testing clay-based composites in various applications could enhance their utility [17]. Technological advancements and method optimizations in clay modification are essential for improving environmental remediation performance, promising innovative solutions for managing aflatoxin contamination and other challenges [8].

6.4 Environmental and Ecological Considerations

Modified clays in environmental remediation offer opportunities and challenges from an ecological perspective. Clays like montmorillonite, bentonite, and zeolite are favored for aflatoxin remediation due to their abundance, biocompatibility, and adsorption capacity, providing a sustainable alternative to chemical methods. Large-scale deployment of biocompatibly functionalized nanoclays requires evaluation of environmental impacts, particularly ecosystem interactions, chemical activity mechanisms, and implications for mineral cycles and colloidal aggregation [7, 10, 18].

Modified clays reduce reliance on chemical pesticides and fertilizers, which pose ecological risks. Biocompatibly functionalized nanoclays enhance remediation efforts, leveraging clays' size-selective permeability and mechanical robustness to support sustainable agricultural practices that protect biodiversity, improve soil health, and minimize chemical runoff [9, 7, 10, 29]. By adsorbing and neutralizing aflatoxins, clays mitigate toxin impacts on ecosystems, promoting healthier soil and water quality. Their natural origin aligns with green chemistry principles, minimizing synthetic compound introduction.

However, the ecological footprint of clay mining and modification warrants evaluation. Unsustainable extraction and processing can disrupt habitats, cause soil erosion, and pollute water. Disposal of spent clays with contaminants poses environmental risks if mismanaged. Sustainable management frameworks for clay resources are essential to mitigate these impacts [16].

The deployment of modified clays raises considerations about interactions with non-target organisms. While generally biocompatible, clays' impact on soil microbiota and plant health should be assessed to avoid unintended ecological consequences. The potential of modified clays, like nanosulfur-bentonite composites, to influence soil pH, nutrient availability, and microbial communities highlights the need for comprehensive ecological studies to ensure their application does not disrupt ecosystems, especially in nutrient cycling and remediation [7, 10, 29, 23].

Emerging trends in remediation emphasize personalized approaches and ethical considerations in deploying technologies like AI to optimize clay modification and application processes. Developing data governance frameworks and integrating ecological feedback mechanisms can enhance the sustainability and effectiveness of clay-based remediation strategies [16].

6.5 Integration with Broader Remediation Strategies

Integrating modified clays into broader remediation strategies requires leveraging their unique properties to address various contaminants. The adsorption and biocompatibility of natural clays, including montmorillonite, bentonite, and zeolite, make them effective components in strategies targeting organic and inorganic pollutants. Modified nanoclays, particularly biocompatibly functionalized ones, enhance remediation efforts by improving contaminant interactions and facilitating innovative pollution management solutions [7, 10].

Combining clay-based adsorption techniques with biological and chemical methods can enhance remediation effectiveness by merging biocompatibly functionalized nanoclays' advantages with other innovative methods, improving contaminant removal and promoting sustainable practices [7, 10, 15, 14]. For instance, using clays with microbial degradation processes can facilitate complex organic pollutant breakdown, while chemical treatments can modify clay surfaces for specific contaminant adsorption.

Advanced computational models, like the Neural Network Potential (NNP), offer potential for optimizing clay integration into broader remediation strategies. Extending NNP training to include zeolites with heteroatoms and guest molecules can enhance applicability to real-world synthesis conditions, allowing tailored clay-based material design for specific remediation needs [31]. This capability is crucial for developing customized solutions for unique environmental challenges.

Incorporating modified clays into existing infrastructure, such as wastewater treatment plants and agricultural systems, offers scalable and cost-effective solutions for mitigating environmental contamination. Clays' capacity, particularly modified nanoclays, to adsorb various pollutants, along with biocompatible functionalization, positions them as promising solutions for improving contemporary remediation practices. Recent research highlights the mechanical robustness and size-selective permeability of clay vesicles, enhancing microcompartmentalization and facilitating targeted contaminant removal in various aqueous environments [7, 10].

7 Conclusion

This survey highlights the critical importance of modified clays, such as montmorillonite, bentonite, and zeolite, in addressing the challenge of aflatoxin contamination. These materials exhibit unique adsorption properties that facilitate the effective sequestration and removal of aflatoxins, driven by their distinct structural and chemical characteristics. Enhancements in adsorption efficiency are achieved through various modification techniques, including chemical, physical, and biological methods, while the application of machine learning and computational modeling further refines these processes. The practical application of nanosulfur-bentonite composites and zeolite-based oxide coatings underscores the potential of these materials in real-world environmental remediation scenarios.

Moreover, the integration of zeolite into polyaniline blends reveals promising opportunities for the advancement of electronic and structural properties in clay-based materials, suggesting new directions for research and development. Continued exploration is essential to enhance our understanding and effectiveness of modified clays in aflatoxin mitigation. Future research should focus on overcoming challenges related to scaling and standardization, developing innovative synthesis and characterization techniques, and embedding modified clays within comprehensive environmental remediation frameworks. Progress in these areas is crucial for devising more effective and sustainable strategies to combat aflatoxin contamination, ultimately safeguarding public health and preserving environmental integrity.

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