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NANOMATERIALS FOR WATER PURIFICATION: THEORETICAL INSIGHTS FROM DENSITY FUNCTIONAL THEORY STUDIES

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Abstract: Nanomaterials have emerged as promising solutions for the removal of various pollutants (such as organic compounds, heavy metals, dyes) from water, with enhanced selectivity, efficiency, and sustainability. This review examines various nanomaterials used in water purification, including metal-based nanoparticles (silver, iron oxide) and carbon derived materials (graphene, carbon nanotubes) for wastewater treatment. Density Functional Theory (DFT) has proven invaluable in providing theoretical insights supplementing the experimental studies. This review highlights how DFT simulations contribute to the understanding of nanoparticle interaction with the pollutant, providing a deeper, fundamental understanding of the chemical and physical processes involved in water purification. DFT studies also provide crucial insights for designing new and improved nanomaterials tailored for wastewater treatment systems. The review also discusses the adsorption mechanisms of nanomaterials for water purification and the key factors influencing their performance. The combination of DFT studies with experiments not only predicts modified material properties but can also provide theoretical guidance for material design. This enhances the scientific validity and reliability of research conclusions. Thus, integrating DFT with experimental studies can accelerate the development of efficient, sustainable, and cost-effective water purification technologies.

IndexTerms - Nanomaterials; Water purification; Density Functional Theory (DFT); Adsorption mechanisms; Metal-based nanoparticles; Graphene; Wastewater treatment; Computational modeling

1. INTRODUCTION

Water is essential for life; however, the ongoing degradation of water systems continues to threaten life on earth. Industries, primarily pharmaceuticals and agriculture, contribute to the degradation with their practice of abstracting and polluting water with difficult to eradicate contaminants like herbicides, phenolic compounds, textile production dyes, and poisonous metal ions. Today's water purification systems are both inefficient and energy intensive. Purification systems that are being developed to treat waste at a lower cost and energy are using nanomaterials, as they are more effective and energy efficient. Metal based nanomaterials like silver, iron oxide, doped titanium dioxide, and other heteroatoms are popular due to their combination of strong absorptive and photocatalytic properties. These properties enhance catalytic transformations as well as adsorptive elimination of target contaminants. However, several persistent issues limit the potential of engineered nanomaterials such as inadequate understanding of contaminant–nanomaterial interactions and their small size and high reactivity can lead to unpredictable interactions with ecosystems, including bioaccumulation, long-term toxicity.

DFT can be used as a reliable and conceptually sound technique for the examination and prediction of various contaminants and their interaction and related the reaction mechanisms involved in contamination and remediation processes. Moreover, DFT is a widely used computational quantum mechanical modeling method to analyze the electronic structure.

This paper gives an overview of the experimental and theoretical work related to nanomaterials used in water purification, with special emphasis on the insights offered by Density Functional Theory. It briefly discusses few mechanisms such as adsorption, photocatalysis, and pollutant–nanomaterial interactions, and discusses how DFT predictions complement empirical findings. The review also highlights the limitations, environmental considerations, and future research perspectives needed for developing safe, efficient, and sustainable nanomaterial -based water treatment technologies.

2. LITERATURE REVIEW

2.1 Nanomaterials in Water Purification

Metal-based nanoparticles have been investigated for some time for their properties such as photo degradation, catalysis, and their particular interactions with microbes and dyes. Their beneficial interactions permit their use in pollutant removal, for example silver nanoparticles have practical applications in various remediation processes. Their ability to remove and concentrate heavy metals is another example where cylindrical and functionalized iron oxide magnetic nanoparticles have been proven to be highly effective due to their mesoporous structure and ease of recovery [1].

Titanium dioxide, are known for their strong photocatalytic properties, which allow them to degrade numerous organic pollutants when exposed to UV and visible light. Carbon-based advanced materials such as graphene and its derivatives have many practical applications currently. They have very large specific surface area, extreme chemical stability, and are able to be modified with oxygenated functional groups. These properties of carbon based nanomaterials are useful in achieving high efficiency for adsorption of diverse compounds, such as pharmaceuticals and dyes, and even metal ions.

2.2 DFT Contributions to Understanding Nanomaterial Reactivity

DFT simulations have substantially advanced the understanding of pollutant–nanomaterial interactions. For instance, Rangel-Vázquez *et al.* reported that functionalization of graphene with modified groups significantly alters its electronic structure, supporting the broader understanding that surface functional groups increases adsorption through hydrogen bonding and electron-donor interactions [2]. DFT has provided knowledge concerning the presence of defect sites within the aggregates of TiO_2, which increases photocatalytic activity through the lowering of the energy barrier required for the degradation of a pollutant, is also available.

DFT has aided in the understanding of the mechanisms of charge transfer, which determines the adsorption strength and, consequently, the activity of the catalyst. For instance, García-Rollán *et al.* have discussed that the oxidation and surface modification of nanomaterials changes their surface charge distribution and introduces additional active sites which improves the adsorption of pollutant through electron redistribution-driven interactions [3]. The use of DFT modelling alongside empirical methods has further strengthened the reliability of predicted material behaviors.

While experimental analysis provides essential macroscopic insight, DFT offers atomistic-level understanding that is rarely accessible through laboratory techniques alone. Several studies have shown close agreement between experimentally measured adsorption efficiencies and DFT-predicted adsorption energies, reinforcing the predictive value of theory. For example, Singh et al. synthesized a GO/UiO-66-NDC MOF nanocomposite for Cr (VI) removal and reported through their DFT simulations that the nanocomposite possessed enhanced delocalized surface states, which significantly increased its adsorption behavior in agreement with experimental trends. Such integrated DFT–experimental studies demonstrate how theoretical screening can reliably identify and explain the superior performance of advanced adsorbent materials [4].

3. METHODOLOGY

3.1 Theoretical Framework

This review compiles information from various DFT-based studies regarding the interaction of nano-materials with water pollutants. The use of GGA with PBE functional to model exchange-correlation energies is the most common approach in the literature. For most studies concerning nanosystems, pseudopotentials and plane wave basis sets are the standard approximations used to describe electron density.

When using DFT for quantum mechanical modeling of materials, researchers works with nanoscale clusters or periodic structures of materials such as graphene oxide, carbon nanotubes, metal oxides, and silver nanoparticles. The contaminants of interest are primarily heavy metals (Pb^{2+}, Cd^{2+}), aromatic organic dyes (e.g., methylene blue), and organic pollutants (e.g., phenol), are subjected to geometry optimization before running adsorption calculations. Standard inputs for such simulations often include:

- Full positive-definite geometry optimization;
- Calculation of adsorption energies (E_{ads});
- Charge transfer (if any) detection using Mulliken or Bader methods;
- Review of Density of States (DoS) and Band structure;
- Frontier molecular orbital (FMO) analysiswhich includes Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) to understandelectronic transition behavior and reactivity.

3.2 Assessment of Interaction Mechanisms

Adsorption mechanisms are studied by identifying adsorption sites, energy calculations required to bind the adsorbate, and monitoring the transfer of charge across the interface. The energies are with a few dominant interactions, which are considered to be the primary mechanisms, including hydrogen bonding, π-π stacking, electrostatic interactions, coordination of metal ions with ligands, and surface defect interactions.

3.3 Validation through Experimental Correlation

The predictive ability of DFT is established by comparing various indicators such as adsorption capacity, degradation rate, and photocatalytic efficiency with experimental results. Discrepancies between experimental and DFT modelling results are of no particular importance. Instead, the scientific community appreciates the indispensable role of DFT in understanding nanoscale interactions and modelling nanoscale systems for high-performance purification materials.

4. DISCUSSION

How do carbon-based nanomaterials respond across differing real-world scenarios? Through the lenses of DFT, this phenomenon is examined. There is a significant increase in the adsorptive capacity of these materials when they undergo functionalization and/or defect engineering. As a result of the emergence of active sites, the electrostatic interactions are

strengthened [5]. The strong empirical performance of these DFT designed metal nanoparticles in purification systems is due to their strong binding to pollutant molecules. DFT explains and predicts this behavior by examining the electron structure and band changes; modification through vacancy engineering in a structure can also be explained [6].

With modifications in these areas, the band gap is reduced, charge separation is improved, and photocatalytic activity is enhanced. There is a portrayal of charge density changes attributed to DFT that reflect the shifts in electron location and pollutant capture at the atomic interfaces. For example: DFT improvements, particularly the nitrogen-doping of graphene accurately predicted varying efficiencies in the removal of pollutants [7]. The correlation of design modifications and improved experimental results further confirms the application of DFT in enhancing materials.The synergy of empirical and theoretical methods provides ample confidence in predicting enhanced material design, as shown in this case.

5. ADSORPTION

In general, adsorption is the process in which dissolved substances accumulate at an interface, where contaminants attach to the surface of water-insoluble adsorbent pores. The extent of adsorption depends on the physicochemical interactions between the adsorbent and the adsorbate at their interface.

Adsorption differs from absorption, where molecules penetrate into the bulk of the material rather than remaining on the surface. Thus, adsorption is a surface-based phenomenon, while absorption involves the entire volume of the material. Because of its simplicity, efficiency, and versatility, adsorption is widely used for pollutant removal.

Adsorption treatment for removal of pollutants from wastewater using nanomaterials could be one of the best physical treatment strategies due to the high specific surface area of the adsorbents [8]. The adsorption process design allows effective removal of contaminants from wastewater. Moreover, it is cost-effective, efficient, and an excellent physical method for removing antibiotics-related contaminants and other pharmaceuticals from wastewater [9]. Nanomaterials, owing to their unique features such as size-dependent properties, large surface area, high degree of functionalization, and affinity to bind positive or negative contaminants, are considered excellent for the removal of toxic contaminants from wastewater [10].

DFT can predict adsorption energies. These energies can be useful for designing materials with specialized qualities for specific uses. DFT with molecular dynamics simulations can be used for investigating the behavior of nanoparticles in complex environments, such as wastewater treatment scenarios, where different solutes and conditions are present [11, 12].

5.1 CASE STUDIES DEMONSTRATING NANOMATERIAL EFFICIENCY

5.1.1 Graphene Oxide for Heavy Metal Removal

Experimental research shows unprecedented and noteworthy adsorption of Pb^{2+} and Cd^{2+} ions by graphene oxide (GO) and is attributed to the availability of plentiful oxygen functional groups [13]. DFT calculations indicate that the carboxyl, hydroxyl, and epoxy groups amplify the binding through strong coordination and charge transfer, effectively weakening the metal–ligand bonds. The theoretical results correlate well with the experimental removal efficiencies, which were markedly high for batch and column studies [14].

5.1.2 Iron Oxide Nanoparticles for Wastewater

In recent years, Fe_2O_3 nanoparticles have attracted considerable interest in textile-related wastewater treatment because of their strong ability to capture and degrade dye molecules. Studies on α-Fe_2O_3 highlight its effective photocatalytic breakdown of textile dyes, a process that can be further enhanced through ultrasound-assisted activation, which increases radical generation and accelerates chromophore destruction [15]. These observations are consistent with broader evaluations of Fe_2O_3 photocatalysts, which report that Fe–O surface sites readily participate in electron transfer processes that weaken dye chromophores and promote their degradation under light or catalytic conditions [16].

Complementary DFT and experimental work comparing CuO with CuO–Fe_2O_3 composites also shows that incorporating Fe_2O_3 modifies the surface electronic structure in a way that strengthens dye adsorption and facilitates electron-driven decomposition pathways, further confirming the central role of Fe–O interactions in dye removal [17]. In addition to their catalytic activity, the magnetic recoverability of Fe_2O_3-based materials allows for easy separation after treatment, improving operational efficiency and reducing the risk of secondary contamination.

5.2 PHOTOCATALYTIC PROCESSES

Photocatalzsis is a light-driven process that utilizes catalysts to accelerate chemical reactions. It is widely used in wastewater treatment and management. The photocatalytic process offers many advantages such as the degradation of pollutants and not just removal. This method utilizes solar energy to break down pollutants into harmless substances, such as CO_2 and water, making it both sustainable and energy-efficient. It does not require any chemical additives and possesses antimicrobial properties. Some photocatalysts, such as Ag, TiO_2, generate reactive oxygen species under light, which effectively kill pathogens. This characteristic is not common in other wastewater treatment mechanisms [18, 19]. Metal-based nanoparticles, such as silver (Ag NPs) and titanium dioxide (TiO_2 NPs), which are influenced by factors like pH, organic matter, and redox conditions, exhibit distinct behaviors in adsorbing, degrading, or transforming pollutants [20]. Ag NPs and TiO_2 NPs primarily act through antimicrobial activity and photocatalytic degradation; their effectiveness depends on their size and shape.

5.2.1 Silver Nanoparticles for Microbial and Chemical Pollutants

Silver nanoparticle (Ag NPs) technology exhibits two major capabilities: efficient microbe biocontrol and chemical absorptive properties [21]. Ag NPs can break down microbial cell membranes and produce reactive oxygen species, which makes them useful for treating wastewater contaminated with pathogens [22]. In addition to their strong antimicrobial and catalytic properties, Ag NPs are highly sensitive, have low detection limits, and can be reused [23]. Sidorowicz et al. in their introduced introduced a new method for dye degradation using Ag NPs with improved photocatalytic activity under visible light. This makes them more useful for real-world environmental cleanup [24].

6. CHALLENGES AND LIMITATIONS

Although nanomaterials hold an abundance of advantages when treating wastewater, some scientific, technological, and ecological concerns still exist and limit the use of nanomaterials on larger scales. One concerns the stability of nanomaterials in heterogeneous aqueous solutions. A number of nanoscale materials, particularly metal-based nanoparticles, are known to become reactive. Furthermore, they lose reactivity and are difficult to recover after treatment, due to dissolution, aggregation, and/or surface oxidation. In addition, the environmental risks can arise from the deliberate release of engineered nanomaterials . Numerous studies have shown that some types of nanoparticles can have toxic impacts on aquatic microorganisms and modify the microbial communities that are vital to different biogeochemical cycles.

While there are useful DFT simulations within methodological considerations, the expense of DFT simulations along with the assumptions of idealized models creates limitations to what can be achieved. The majority of DFT studies assume vacuum or idealized solvent conditions, which ignores the complex chemistry of real-world wastewater systems. Furthermore, the simulations of large biomaterials, or composite materials, or the simultaneous interactions of multiple pollutants, tend to require substantial amounts of computational power, thus exacerbating the gap between simplified theoretical models and complex real-world systems [25]. Given the need for the innovative expansion of these computational methods, the materials stability needs to be improved, along with a more comprehensive evaluation of the environmental impacts.

7. FUTURE RESEARCH PERSPECTIVES

A multi-tier approach is essential in researching nanomaterials and their integration with water purification technologies. One of the main focuses could be the creation of hybrid multifunctional nanomaterials with the ability of adsorption, catalysis, and anti-microbial in one unit. These materials would add functionality and therefore, reduce losses on contaminant retention through other mechanisms. Lately, two major lines of research have emerged. One involves the integration of machine learning (ML) and artificial intelligence (AI), most effectively when combined with density functional theory (DFT) data.

The target is to make the materials development cycle faster with the above methods. ML for instance, can be employed to estimate adsorptionenergy and then fit a DFT-calculated data set to within the model. ML would be beneficial if thousands of nanomaterials with low experimental feasibility could be screened prior to moving to the lab.Besides, the focus to develop green technologies and their potential impact has expedited the creation of non-toxic and biodegradable nanomaterials [26]. One can adopt eco-friendly methods for nanoparticle synthesis using plants, for carbon materials using biomass, or with nanostructures of other naturally found minerals. The advanced DFT is expected to play a significant role in the prediction of the developed nanomaterials on their stability, reactivity, pollutant-binding and overall, on sustainable efficiency.

8. APPLICATIONS IN REAL-WORLD WATER TREATMENT SYSTEMS

For municipal, rural, and industrial applications, the real world water treatment systems utilize photocatalytic, dye, pathogen, and pharmaceutical removal technologies and enhancements. For decentralized water purification systems, metal oxides enhanced with graphene have demonstrated a high degree of removal of recalcitrant contaminants, particularly those associated with industrial textiles and chemicals, under both visible and ultraviolet radiation. Improvements based upon DFT have already had some effect on systems in commercial use today. Silver (Ag) doping in titanium dioxide (TiO_2) photocatalytic self-cleaning water treatment reactors has enhanced photocatalytic activity [27]. In a similar fashion, theoretically based design of graphene oxide membranes, in terms of pore size and charge configuration, has excelled in the adsorption and removal of dyes from water in pilot applications [28]. The successful progression from theory to laboratory to practical applications underlines the equally vital nature of the theory and the supporting experimental and engineering designs.

9. ENVIRONMENTAL AND ECONOMIC CONSIDERATIONS

Pollutant removal is one of the many capabilities of nanomaterials, however, distance, cost, and remote impacts should be considered for their sustainable use. The cost of some nanoparticles is quite high for large-scale use, especially if their synthesis is economically infeasible, as it needs a lot of energy and it is expensive to regulate the synthesis conditions [29]. The economically viable large-scale synthesis procedures such as sol-gel synthesis, or the biological synthesis of nanoparticles, should be developed to economically support the large-scale synthesis procedures [30]. Though nanomaterials offer a complete pollutants removal, their future impacts must be carefully considered alongside economic viability to ensure truly sustainable application.

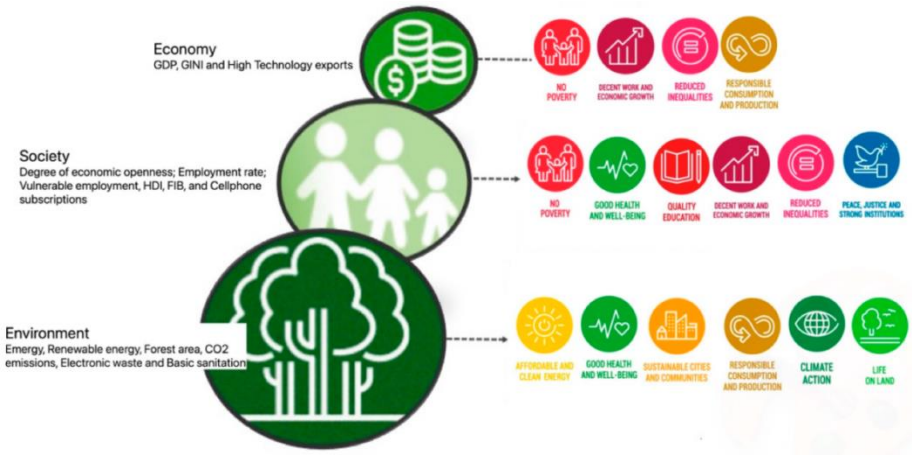

*Image Reference: [31]

Figure1. Showing the Image Environmental and Economic Considerations

10. TOXICOLOGICAL AND ENVIRONMENTAL SAFETY OF NANOMATERIALS

The use of engineered nanomaterials being deployed to treat contaminated water and their environmental and biological effects, raise concerns. Silver and iron oxide engineered nanomaterials are metallic and highly soluble pollutants, and can be problematic due to the leaching of metal ions into water that can cause oxidative stress to microorganisms and other aquatic life. Carbon nanomaterials, more specifically graphene, and carbon nanotubes, are believed to diffuse across cellular membranes to cause cellular hyperventilation and other metabolic disturbances. The above mentioned concerns justify the more complete examination of these nanostructures with particular emphasis on the selective (specific) toxicology and the cellular and/or ecological interactions. Modeling the interactions between biomolecules and engineered nanomaterials such as proteins, cellular membranes and nucleic acids (RNA and DNA) utilizing the Density Functional Theory (DFT) method enables the prediction of the toxicity of the engineered nanomaterials [32]. In silico predictions which focus on the charge density of a nanomaterial are indicative of a wide spectrum of toxicity, ranging from oxidative stress to disruption of membranes.These engineered nanomaterialaccording to theoretical predictions, are less toxic, are biocompatible and less responsive to harmful environmental changes. Moreover, toxicologically optimized engineered nanomaterials are designed to comply with the world's first engineered nanomaterial regulation which targets the sustainable treatment of water for pollution remediation.

11. CONCLUSION

Nanomaterials demonstrate significant potential in advancing water treatment owing to their efficiency, selectivity, and tunable structural and electronic properties. Their ability to eliminate diverse pollutants—including heavy metals, organic dyes, pharmaceuticals, and pathogens—highlights their broad applicability. This review shows how Density Functional Theory (DFT) forms the essential theoretical foundation for understanding atomic-scale interactions, explaining why certain nanomaterials exhibit enhanced reactivity, charge transfer, and adsorption behavior. DFT also provides predictive capability for designing doped or modified materials with superior pollutant-binding characteristics. Although the complexity of real wastewater environments and the limitations of idealized DFT models pose challenges, integrating DFT with experimental validation strengthens material design and improves reliability. In future combining nanotechnology with DFT-based modeling will be crucial for developing economical, sustainable, and high-performance purification systems. Ongoing research is continually validating this approach, leveraging computational power to unlock the potential of advanced materials for water treatment technologies**.**

REFERENCES

[1] Gong, Z., Chan, H. T., Chen, Q., & Chen, H. 2021. *Application of Nanotechnology in Analysis and Removal of Heavy Metals in Food and Water Resources*. **Nanomaterials**, 11(7): 1792.

[2] Olawade, D. B., Wada, O. Z., Fapohunda, O., Egbewole, B. I., Ajisafe, O., & Ige, A. O. 2024. *Nanoparticles for microbial control in water: Mechanisms, applications, and ecological implications*. **Frontiers in Nanotechnology**, 6: 1427843.

[3] Rangel-Vázquez, N. A., Bonilla-Petriciolet, A., Márquez-Brazón, E. A., Huerta, Y., Zavala-Arce, R., & Rodríguez-Macías, J. D. 2025. *DFT-Based Functionalization of Graphene with Lithium-Modified Groups for Enhanced Hydrogen Detection: Thermodynamic, Electronic, and Spectroscopic Properties*. **Nanomaterials**, 15(16): 1234.

[4] García-Rollán, M., Sanz-Santos, E., Belver, C., & Bedia, J. 2025. *Key adsorbents and influencing factors in the adsorption of micro- and nanoplastics: A review*. **Journal of Environmental Management**, 383: 125394.

[5] Singh, S., Anil, A. G., Uppara, B., et al. 2024. *Adsorption and DFT investigations of Cr(VI) removal using nanocrystals decorated with graphene oxide*. **npj Clean Water**, 7: 17.

[6] Raizada, P., Soni, V., Kumar, A., Singh, P., Khan, A. A. P., Asiri, A. M., Thakur, V. K., & Nguyen, V.-H. 2021. *Surface defect engineering of metal oxides photocatalyst for energy application and water treatment*. **Journal of Materiomics**, 7(2): 388–418.

[7] Geldasa, F. T., & Dejene, F. B. 2025. *Effects of S Doping and Oxygen Vacancy on the Physical Properties of Rutile TiO_2 for Photocatalysis Applications Based on Density Functional Theory Study*. **Materials**, 18(8): 1688.

[8] Srivastava, M., & Srivastava, A. 2021. *DFT analysis of nitrogen and boron doped graphene sheet as lead detector*. **Materials Science and Engineering B**, 269: 115165.

[9] Ahmed, S. F., Mofijur, M., Nuzhat, S., Chowdhury, A. T., Rafa, N., Uddin, M. A., Inayat, A., Mahlia, T. M. I., Ong, H. C., Chia, W. Y., & Show, P. L. 2021. *Recent developments in physical, biological, chemical, and hybrid treatment techniques for removing emerging contaminants from wastewater*. **Journal of Hazardous Materials**, 416: 125912.

[10] Riaz, L., Anjum, M., Yang, Q., Safeer, R., Sikandar, A., Ullah, H., Shahab, A., Yuan, W., & Wang, Q. 2020. *Treatment technologies and management options of antibiotics and AMR/ARGs*. **Antibiotics and Antimicrobial Resistance Genes in the Environment**, Elsevier.

[11] Ugwoke, E., Aisida, S. O., Mirbahar, A. A., Arshad, M., Ahmad, I., Zhao, T. K., & Ezema, F. I. 2020. *Concentration-induced properties of silver nanoparticles and their antibacterial study*. **Surfaces and Interfaces**, 100419.

[12] Penna, M. J., Mijajlovic, M., & Biggs, M. J. 2014. *Molecular-level understanding of protein adsorption at the interface between water and a strongly interacting uncharged solid surface*. **Journal of the American Chemical Society**, 136: 5323–5331.

[13] Wonglakhon, T., Chonsakon, A., Nuengmatcha, P., Ninwong, B., Zahn, D., & Thepchuay, Y. 2025. *Green Synthesized Silver Nanoparticles from Biowaste for Rapid Dye Degradation: Experimental Investigation and Computational Mechanistic Insights*. **Molecules**, 30(18): 3738.

[14] Joshi, N. C., & Gururani, P. 2022. *Advances of graphene oxide-based nanocomposite materials for treatment of wastewater containing heavy metal ions and dyes*. **Current Research in Green and Sustainable Chemistry**, 5: 100306.

[15] Sun, M., Li, P., Jin, X., Ju, X., Yan, W., Yuan, J., & Xing, C. 2018. *Heavy metal adsorption onto graphene oxide and amino-functional magnetic nanoadsorbents, and application for detection of Pb(II)*. **Food and Agricultural Immunology**, 29(1): 1053–1073.

[16] Gobouri, A. A. 2016. *Ultrasound enhanced photocatalytic properties of α-Fe_2O_3 nanoparticles for degradation of dyes*. **Research on Chemical Intermediates**, 42: 5099–5113.

[17] Hitam, C. N. C., & Jalil, A. A. 2020. *A review on exploration of Fe_2O_3 photocatalyst towards degradation of dyes and organic contaminants*. **Journal of Environmental Management**, 258: 110050.

[18] Al-Garawi, Z., Ismail, A., Hillo, D., Öztürkkan, F., Necefoğlu, H., Mohamed, G., & Abdallah, A. 2024. *Experimental and density functional theory studies on metal oxides and derived nanoclusters: comparative effects on human ferritin*. **Discover Nano**, 19.

[19] Abebe, B., Murthy, H. C. A., & Amare, E. 2018. *Summary on adsorption and photocatalysis for pollutant remediation: Mini review*. **Journal of Encapsulation and Adsorption Sciences**, 8: 225–255.

[20] Martínez, G., Merinero, M., Pérez-Aranda, M., Pérez-Soriano, E. M., Ortiz, T., Begines, B., & Alcudia, A. 2021. *Environmental impact of nanoparticles' application as an emerging technology: A review*. **Materials**, 14: 166.

[21] Bundschuh, M., Filser, J., Lüderwald, S., McKee, M. S., Metreveli, G., Schaumann, G. E., Schulz, R., & Wagner, S. 2018. *Nanoparticles in the environment: where do we come from and where do we go?* **Environmental Sciences Europe**, 30: 1–17.

[22] Dhaka, A., Mali, S. C., Sharma, S., & Trivedi, R. 2023. *A review on biological synthesis of silver nanoparticles and their potential applications*. **Results in Chemistry**, 6: 101108.

[23] Krishna, S. B. N., Sheik, A. G., Pillay, K., Hamza, M. A., Elamir, M. Y. M., & Selim, S. 2024. *Nanotechnology in action: silver nanoparticles for improved eco-friendly remediation*. **PeerJ**, 12: e18191.

[24] Sidorowicz, A., Fais, G., Desogus, F., et al. 2024. *Optimization of Brilliant Blue R photocatalytic degradation by silver nanoparticles synthesized using Chlorella vulgaris*. **Environmental Science and Pollution Research**, 31: 57765–57777.

[25] Minervino, A., & Belfield, K. D. 2024. *Review of Recent Computational Research on the Adsorption of PFASs with a Variety of Substrates*. **International Journal of Molecular Sciences**, 25(6): 3445.

[26] Liu, Y., Esan, O. C., Pan, Z., & An, L. 2021. *Machine learning for advanced energy materials*. **Energy AI**, 3: 100049.

[27] Zarzecka, C., Goldoni, J., Oliveira, J. P., Lenzi, G. G., Bagatini, M. D., & Colpini, L. M. S. 2024. *Photocatalytic action of Ag/TiO_2 nanoparticles for degradation of emerging pollutants: A comprehensive review*. **Sustainable Chemistry for the Environment**, 8: 100177.

[28] Alnoor, O., Laoui, T., Ibrahim, A., Kafiah, F., Nadhreen, G., Akhtar, S., & Khan, Z. 2020. *Graphene Oxide-Based Membranes for Water Purification Applications: Effect of Plasma Treatment on the Adhesion and Stability of the Synthesized Membranes*. **Membranes**, 10(10): 292.

[29] Ghosh, A., Chakraborty, R., Das, A., et al. 2024. *Abating air pollution using nanoparticles and sustainable technologies through a holistic lens*. **Nanotechnology for Environmental Engineering**, 9: 637–677.

[30] Ying, S., et al. 2022. *Green synthesis of nanoparticles: Current developments and limitations*. **Environmental Technology & Innovation**, 26: 102336.

[31] Terra dos Santos, L. C., Frimaio, A., Giannetti, B. F., Agostinho, F., Liu, G., & Almeida, C. M. V. B. 2023. *Integrating environmental, social, and economic dimensions to monitor sustainability in the G20 countries*. **Sustainability**, 15(8): 6502.

[32] Zhang, X.-Q., Xu, X., Bertrand, N., Pridgen, E., Swami, A., & Farokhzad, O. C. 2012. *Interactions of nanomaterials and biological systems: implications to personalized nanomedicine*. **Advanced Drug Delivery Reviews**, 64(13): 1363–1384.