

Quantum Computing for Carbon Capture and Reduction: An Analysis of the Technological Frontiers

Natalia Fernanda Silva Vilas Boas^{1*}, Victor Menezes Vieira², Sergio Luis Costa Ferreira³

¹ Senai Cimatec University, Environmental Area, Salvador, Bahia, Brazil

² Senai Cimatec, Environmental Area, Salvador, Bahia, Brazil

³ Senai Cimatec University, Chemistry Area, Salvador, Bahia, Brazil

*Corresponding author: Senai Cimatec University; Orlando Gomes Ave. 1845 (Piatã), Salvador, BA, 41650-010; natalia.fernanda@fbter.org.br

Abstract : This study presents a systematic review of the applications of quantum computing in atmospheric carbon capture and reduction technologies, investigating how this disruptive technology can revolutionize climate mitigation efforts. The bibliometric analysis revealed an exponential growth in publications concentrated between 2020 and 2025 (86.5% of the total), led by the United States (18.9%), followed by the United Kingdom (15.5%) and China (12.1%), highlighting the leading role of developed economies. Energy and Engineering lead with 13.9% each, followed by Chemistry and Computer Science (12.7% each), demonstrating the interdisciplinary nature of the field. The main results identified four transformative technologies: advanced molecular simulations using VQE and DMET algorithms for optimization of Metal-Organic Frameworks with relative error below 0.2%; optimization of energy systems with reductions of up to 30% in consumption through quantum algorithms; Enhanced climate modeling with quantum machine learning algorithms, achieving sensitivity of up to 80% in extreme event predictions; and the development of materials such as RM/CaO adsorbents with capacities of 0.481 g/g of CO₂ and high cyclic stability. One study projects the potential to eliminate more than 7 gigatons of CO₂ equivalent annually by 2035, representing a cumulative reduction of over 150 gigatons over the next 30 years if quantum applications are used to facilitate the removal of CO₂ from the atmosphere. However, critical gaps were identified in computational scalability, with runtimes limiting practical applications, experimental validation revealing substantial differences between theoretical simulations and real hardware, the need for standardized frameworks for industrial integration, and the development of specialized quantum architectures for environmental applications. The study concludes that quantum computing constitutes an imperative technological need to address contemporary climate challenges, positioning itself as a priority for research and development investments.

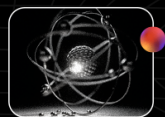
Keywords: Quantum Computing, Carbon Capture, Quantum Algorithms, Sustainability, Climate Mitigation

1. INTRODUCTION

Climate change represents one of the greatest challenges of the 21st century, requiring innovative technological solutions to reduce greenhouse gas emissions and achieve carbon neutrality goals [1]. In this context, quantum computing emerges as a disruptive technology capable of revolutionizing several sectors critical to climate mitigation, including carbon capture, energy systems, and the development of sustainable materials [2]. Quantum computing, based on the principles of quantum mechanics such as superposition and entanglement, offers

exponentially superior computational capabilities to solve complex optimization problems that are intractable for classical computers [1]. According to Ashwani et al. (2024), quantum algorithms demonstrate transformative potential in applications related to climate change, especially in energy optimization, improved climate modeling, and weather forecasting [3].

The energy sector, responsible for 81% of the world's commercial energy supply, plays a critical role in the transition to a net-zero emissions future [2]. Integrating quantum technologies into this sector can significantly



accelerate the development and implementation of low-carbon solutions, from optimizing renewable energy systems to enhancing carbon capture and storage technologies [4].

Recent studies demonstrate that quantum computing has the potential to contribute to the removal and sequestration of carbon dioxide at a rate 122% higher than the current rate, representing approximately 7 gigatons of CO₂ equivalent per year by 2035 [1]. This capability is particularly relevant for the development of direct air capture technologies and the improvement of adsorbent materials such as Metal-Organic Frameworks (MOFs) [5-6].

2. METHODOLOGY

This study adopted one review approach systematic literature to analyze the applications of physics quantum in the generation of carbon credits. The methodology followed specific criteria to ensure the quality and relevance of documents analyzed. The research was conducted using the Scopus database (Elsevier). After applying all predefined filters and restrictions, the search returned 21 relevant results. Table 1 summarizes the criteria adopted in the selection process.

Table 1. Scope of research of scientific articles.

SEARCH CRITERIA	
Analysis Period	The research covered the entire time range of publications.
String	("quantum mechanics " OR "quantum physics " OR "quantum computing " OR "quantum algorithms ") AND (" carbon credits " OR " carbon market " OR " carbon finance " OR " carbon emission trading" OR

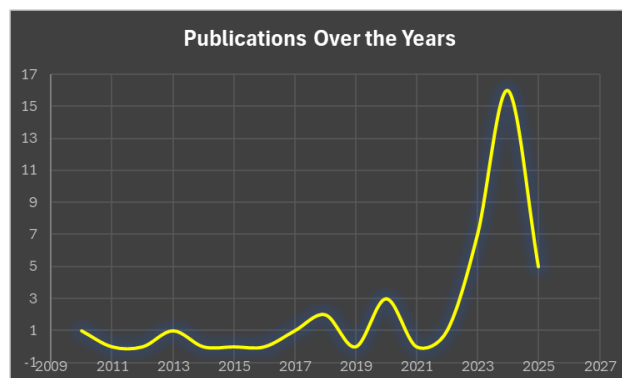
	" carbon offset" OR " carbon capture" OR " climate change mitigation " OR "net zero").
Restrictions	Closed documents or documents that do not jointly address the quantum issue with the issue of carbon capture or emissions reduction.
Keyword Search Area	Title, abstract and keyword.
Document Types	Articles, conference papers and review articles.

3. RESULTS AND DISCUSSION

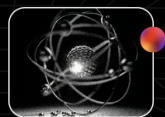
3.1. Bibliometric Analysis

Initially, three analyses were carried out to identify the behavior of scientific publications over the years, which countries are most active and which areas of study have stood out the most, as can be seen in Figures 1, 2 and 3. The temporal analysis of publications shows us a characteristic pattern of emerging research fields (Figure 1).

Figure 1. Number of publications over the years.



The period analyzed (2010-2025) demonstrates relatively modest scientific production. The temporal pattern presents notable characteristics: seven years (2011, 2012, 2014, 2015, 2016, 2019, 2021) recorded zero publications, suggesting a discontinuity in scientific production that may reflect both the technological limitations of the time and the lack of a critical mass of researchers at the intersection of these

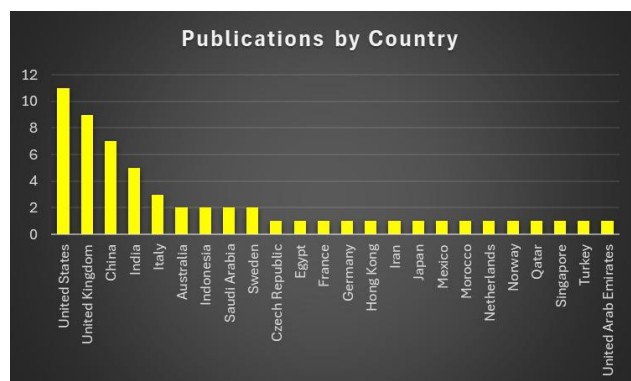


fields. This intermittency is typical of nascent research areas, where conceptual development precedes empirical consolidation.

The exponential growth observed between 2020 and 2025 is particularly significant, accounting for 86.5% of all publications (32 of 37 documents). The peak in 2024, with 16 publications, represents a milestone in the field's scientific production, suggesting a maturation of the field coinciding with recent advances in both quantum computing and carbon capture technologies. The slight reduction to 5 publications in 2025 should be interpreted with caution, considering that the data may be incomplete since the year is not yet over.

Geographical analysis reveals a marked concentration of scientific production in developed economies, with important implications for the democratization of knowledge in this strategic field (Figure 2).

Figure 2. Number of publications by country.



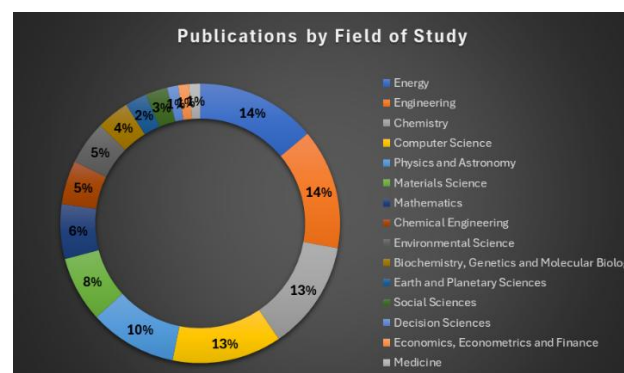
The United States leads with 11 publications (18.9% of the total), followed by the United Kingdom with 9 publications (15.5%) and China with 7 publications (12.1%).

This distribution reflects not only these countries' investment capacity in research and development, but also their established scientific infrastructure in

quantum computing. India's presence in fourth place, with 5 publications, represents a notable development for this country, considering the growth of its technology sector and government investment in quantum technologies. The concentration of the top five countries at 60.3% of total production suggests the existence of significant inequalities in access to quantum technologies and research resources, a factor that could impact the global capacity to develop solutions to climate change.

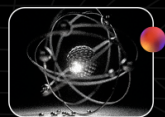
The analysis of the study areas shows us the interdisciplinary nature inherent in the application of quantum computing in capturing and reducing carbon emissions (Figure 3).

Figure 3. Percentage of publications by area of study.



The relatively balanced distribution among the main areas contrasts with the typical concentration of more mature fields, suggesting that this intersection is still in the process of defining disciplinary boundaries.

Energy and Engineering share the lead with 13.9% each, reflecting the field's practical orientation toward applied solutions. This parity suggests a balanced approach between energy fundamentals and technological implementation, essential characteristics for the viability of carbon capture technologies. Chemistry and Computer Science rank second with 12.7% each, highlighting the importance



of both the chemical processes fundamental to carbon capture and the quantum algorithms needed to optimize these processes. This balanced distribution suggests effective integration between computational theory and chemical applications. The significant presence of Physics and Astronomy (10.1%) and Materials Science (7.6%) reinforces the fundamental scientific foundation necessary for the development of applied quantum technologies. The contribution of Mathematics (6.3%) underscores the importance of algorithmic and optimization fundamentals.

Particularly notable is the limited participation of Social Sciences (2.5%) and Economics (1.3%), fields crucial to the practical implementation and economic viability of carbon capture solutions. This gap may represent a strategic limitation in the development of technologies that depend on both technical feasibility and social acceptance and economic sustainability.

3.2. Analysis of Data Presented in the Articles

The analysis revealed several applications of quantum computing in technologies related to carbon credit generation. The studies range from molecular simulations to the optimization of complex energy systems, demonstrating the transformative potential of this technology. It was identified that this scientific field is rapidly expanding, with quantum computing emerging as a transformative tool to address the challenges of atmospheric carbon capture and reduction. The studies demonstrate a convergence between advanced quantum algorithms and critical environmental applications, establishing new paradigms for global sustainability [7].

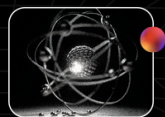
The work of Cheung et al. (2013) and Greene-Diniz et al. (2022) establishes the fundamental theoretical basis for quantum applications in carbon capture. Using the Variational Quantum Eigensolver (VQE) and Density Matrix Embedding Theory (DMET), these studies demonstrated that quantum simulations can optimize Metal-Organic Frameworks (MOFs) for CO₂ adsorption with higher accuracy than classical methods [5, 8].

Specifically, Dahale et al. (2023) reported that DMET-VQE algorithms achieved relative errors of only 0.16×10^{-3} for CO₂ + Cu-MOF-74 systems, significantly outperforming reduced DMET-CCSD methods [6].

Annealing algorithms, as demonstrated by Zhai et al. (2024), revealed exceptional capabilities for carbon emission rights pricing (CERO). The results indicated superior convergence compared to classical Gale-Shapley methods, with a significant reduction in CO₂ emissions during the computational processes, which is a particularly relevant feature for environmental applications [9].

The studies by Cardoso et al. (2025) and Zhu et al. (2025) significantly expand our understanding of molecular interactions in carbon capture systems. Using DFT (Density Functional Theory) integrated with quantum simulations, it was demonstrated that carbon Nitrogen-functionalized dots exhibit exceptional selectivity for 4-nitrophenol, with 98% photoluminescence quenching and a redshift of 34 nm in aqueous media [10-11].

Of particular interest are the results of Shi et al. (2020), who demonstrated how moisture-driven sorbent systems can achieve CO₂ adsorption capacities of



0.481 g/g – representing 171.43% of the capacity of pure CaO. Integration of quantum mechanical simulations revealed that the CO₂ adsorption energetics can be enhanced to -8.25 eV on RM/ CaO (200) crystal surfaces, indicating significantly stronger atomic interactions [12].

The works of Liu & Tang (2023), Celsi & Celsi (2024) and Zhao et al. (2023) established a robust framework for applying quantum computing to power systems. The analysis reveals that quantum algorithms can optimize power flows, unit commitment, and economic dispatch with exponentially higher computational efficiency than classical methods [1, 7, 13].

Specifically, Ashwani et al. (2024) demonstrated that the application of Quantum Random Access Memory (qRAM) and Generative Adversarial Networks can significantly improve grid stability, demand forecasting, and cybersecurity in renewable energy systems. The results indicate reductions of up to 30% in energy consumption through real-time quantum optimization of solar panel alignment [3].

Makhanov et al. 's (2024) investigation into flight trajectory optimization using quantum algorithms reveals substantial potential for reducing emissions in the aviation sector. By implementing Grover's minimum-finding algorithm within Dijkstra 's algorithm, the authors demonstrated improvements of up to 20% in energy efficiency compared to classical optimization methods [14].

Ayaz & Nekovee (2024) expanded these applications to sustainable 6G networks, where QUBO (Quadratic Unconstrained Binary Optimization) optimize bidirectional energy exchange between base stations,

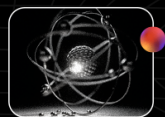
electric vehicles, and the power grid. The results show that quantum approaches produce lower CO₂ emissions compared to classical Gale- Shapley matching algorithms [15].

The studies by Ashwani et al. (2024), Ho et al. (2024), and Dhuliya et al. (2024) demonstrate promising applications of Quantum Machine Learning (QML) for advanced climate modeling. Implementations of Quantum Support Vector Machines (QSVM) and Quantum Convolutional Neural Networks (QCNN) achieved sensitivities of 40% and 80%, respectively, for flood forecasting, significantly outperforming classical methods such as K- Nearest. Neighbors and linear regression (0% sensitivity) [3, 4, 16].

The systematic review by Munawar & Surendro (2024) identified 40 distinct quantum methods applied to urban carbon neutrality, including Quantum Annealing (QA), Quantum- inspired Particle Swarm Optimization (QiPSO), and Quantum Approximate Optimization Algorithm (QAOA). Analysis of 96 papers indicated that allocation and routing tasks dominate applications, with the transportation and energy sectors presenting more mature implementations [17].

The results of Greene-Diniz et al. (2022) and Dahale et al. (2023) set important benchmarks for quantum simulations of carbon capture. Using DMET-based fragmentation with VQE as the fragment solver, it was demonstrated that the adsorption energy of CO₂ on Al- fumarate can be calculated with an accuracy of -8.25 eV, revealing previously inaccessible guest - host binding mechanisms [5-6].

The work of Tian et al. (2025) on RM/ CaO coupled adsorbents reveals saturated CO₂ adsorption



capacities of 0.481 g/g while maintaining high cyclic stability after 15 adsorption-desorption cycles. Quantum mechanical simulations confirmed stronger atomic interactions, with CO₂ adsorption energy enhanced to -8.25 eV on the RM/ CaO (200) crystal surface [18].

Zhu et al. (2025) demonstrate innovative applications of quantum simulations to understand CO₂ adsorption mechanisms in natural deep eutectic solvents (NaDES) containing L-arginine and glycerol. Using molecular dynamics and quantum mechanical calculations, it was revealed that L-arginine functions primarily as a hydrogen bond acceptor, while glycerol serves as a donor, with both contributing to hydrogen bonds that participate in CO₂ binding [11].

Despite promising advances, studies reveal significant limitations in current scalability. Greene-Diniz et al. (2022) report runtimes of ~50 minutes for fragment Hamiltonian calculations, indicating the need for more efficient implementations. Resource estimation shows exponential increases in Hamiltonian terms (from 361 to 14,243) with expansion of the HOMO-LUMO active space [5].

The analysis reveals a critical gap between theoretical simulations and experimental validation on real quantum hardware. Dahale et al. (2023) demonstrate substantial differences between noise-free simulations and hardware runs, with consistently higher relative errors in real hardware runs ($10.0\text{--}33.45 \times 10^{-3}$) compared to noisy simulations ($9.77\text{--}23.29 \times 10^{-3}$) [6].

The papers identify an urgent need for integrated frameworks that combine quantum optimization with practical carbon capture systems. Morstyn & Wang

(2024) highlight that industrial implementations require additional research in: (1) benchmark problem definitions and performance criteria; (2) domain-specific algorithms and hardware for current NISQ devices; (3) holistic energy industry computing strategies integrating quantum computing [19].

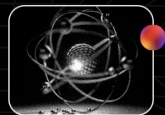
The economic analysis based on the studies reveals transformative potential for cost reduction in carbon capture. Zhai et al. (2024) demonstrate that CERO pricing based on quantum algorithms can reduce operational costs through more efficient price discovery and market risk reduction [9].

Celsi & Celsi (2024) estimates that quantum applications could facilitate the elimination of more than 7 gigatons of CO₂ equivalent annually by 2035, surpassing current trajectories. This would translate into a cumulative reduction of more than 150 gigatons over the next 30 years [1].

Studies indicate the need for investments in specialized quantum infrastructure. Dhuliya et al. (2024) propose a Carbon-aware Quantum Computing model that assesses and reduces the environmental footprint of quantum systems, ensuring compatibility with sustainability objectives [4].

The analysis reveals that the energy sector presents the most mature applications of quantum algorithms for carbon reduction. Liu and Tang (2023) demonstrate that quantum optimization can improve renewable energy penetration, computational efficiency, and help achieve net-zero goals by 2050 [13].

Makhanov et al. (2024) set important precedents for transportation applications, demonstrating that quantum trajectory optimization can reduce fuel



consumption and emissions. Implementations in 6G networks by Ayaz & Nekovee (2024) show the potential for more efficient integrated transportation systems [14].

The work of Tian et al. (2025) and others demonstrates direct industrial applications, where quantum-optimized materials can be implemented in large-scale carbon capture plants [18].

The integration of VQE with classical methods, as demonstrated by Dahale et al. (2023), offers competitive accuracy with limited quantum resources. The analysis identifies a critical need for specialized quantum hardware for environmental applications. The current limitations of NISQ devices require the development of optimized quantum architectures for carbon capture simulations. The studies highlight an urgent need for standardized frameworks for validating quantum algorithms in carbon capture applications, including performance metrics, test protocols, and industrial benchmarks [6].

4. CONCLUSIONS

This analysis showed that quantum computing is emerging as a transformative technology for addressing the climate emergency, such as capturing and reducing carbon emissions from the atmosphere. The results demonstrate superior capabilities of quantum algorithms in multiple areas: optimization of capture materials, climate forecasting, energy management, and sustainable transportation systems. The evidence analyzed indicates the potential to eliminate more than 7 gigatons of CO₂ equivalent annually by 2035, representing a cumulative reduction of more than 150 gigatons over the next 30

years. This impact would position quantum computing as a key technology for achieving global carbon neutrality goals.

The main technologies identified that can significantly contribute to the generation of carbon credits were:

- Advanced Molecular Simulations: VQE and DMET algorithms demonstrated superior accuracy in optimizing MOFs and other capture materials, with adsorption energies calculated with relative error below 0.2%.
- Energy Systems Optimization: Quantum implementations in smart grids show reductions of up to 30% in energy consumption through real-time optimization.
- Improved Climate Modeling: Quantum machine learning algorithms achieve sensitivities of up to 80% in predicting extreme events, significantly outperforming classical methods;
- Emerging Practical Applications: development of materials such as RM/CaO adsorbents with capacities of 0.481 g/g CO₂ and proven cyclic stability.

Regarding the identification of critical gaps and opportunities, the following can be identified:

- Computational Scalability: urgent need for more efficient algorithms for large-scale systems, with execution times currently limiting practical applications;
- Experimental Validation: significant gap between theoretical simulations and implementations in real quantum hardware, requiring more robust validation protocols.



- Industrial Integration: lack of standardized frameworks for integrating quantum solutions into existing carbon capture plants;
- Specialized Hardware: necessary development of quantum architectures optimized for specific environmental applications.

The convergence of evidence presented positions quantum computing not only as a scientific field experiencing clear growth but, also demonstrates it as a fundamental technological opportunity to address contemporary climate challenges. The current scientific momentum, combined with demonstrable practical results, positions this area as a priority for research and development investment in the coming years.

REFERENCES

- [1] Celsi, M. R., & Celsi, L. R. (2024). Quantum Computing as a Game Changer on the Path towards a Net-Zero Economy: A Review of the Main Challenges in the Energy Domain. *Energies*, 17(5), 1-22.
- [2] Ferdous, M. M., Dam, T., Anavatti, S., & Das, S. (2024). Digital technologies for a net-zero energy future: A comprehensive review. *Renewable and Sustainable Energy Reviews*, 202, 114681.
- [3] Ashwani, S., Tripathy, A. J., Karna, S., Jahanve, P. R., & Rajagopal, S. M. (2024). Quantum computing for climate change: A comprehensive review of current applications, challenges, and future directions. In *2024 15th international conference on computing communication and networking technologies (ICCCNT)* (pp. 1-7). IEEE.
- [4] Dhuliya, P., Rana, D. S., Goyal, S., Kukreti, S., & Pundir, S. (2024). Quantum Computing for Sustainable Development: A Framework for Environmental and Social Impact. In *2024 International Conference on Advances in Computing, Communication and Materials (ICACCM)* (pp. 1-7). IEEE.
- [5] Greene-Diniz, G., Manrique, D. Z., Sennane, W., Magnin, Y., Shishenina, E., Cordier, P., ... & Ramo, D. M. (2022). Modelling carbon capture on metal-organic frameworks with quantum computing. *EPJ Quantum Technology*, 9(1), 37.
- [6] Dahale, G. R. (2023). Quantum Simulations for Carbon Capture on Metal-Organic Frameworks. *2023 IEEE International Conference on Quantum Computing and Engineering (QCE)*, 89-93.
- [7] Zhao, N., Zhang, H., Yang, X., Yan, J., & You, F. (2023). Emerging information and communication technologies for smart energy systems and renewable transition. *Advances in Applied Energy*, 9, 100125.
- [8] Cheung, O., Bacsik, Z., Liu, Q., Mace, A., & Hedin, N. (2013). Adsorption kinetics for CO₂ on highly selective zeolites NaKA and nano-NaKA. *Applied Energy*, 112, 1326-1336.
- [9] Zhai, D., Zhang, T., Liang, G., & Liu, B. (2024). Quantum carbon finance: Carbon emission rights option pricing and investment decision. *Energy Economics*, 134, 107628.
- [10] Cardoso, AO, Bogireddy, NKR, Celaya, CA, Muñiz, J., & Agarwal, V. (2025). Experimental and theoretical approaches to uncover the interaction mechanisms of carbon dots with 4-nitrophenol. *Journal of Hazardous Materials*, 485, 136783.
- [11] Zhu, C., Wood, H., Carbone, P., D'Agostino, C., & de Visser, S. P. (2025). CO₂ adsorption in natural deep eutectic solvents: insights from quantum mechanics and molecular dynamics. *Physical Chemistry Chemical Physics*, 27, 2381-2394.
- [12] Shi, X., Xiao, H., Kanamori, K., Yonezu, A., Lackner, K. S., & Chen, X. (2020). Moisture-driven CO₂ sorbents. *Joule*, 4(8), 1823-1837.
- [13] Liu, H., & Tang, W. (2023). Quantum computing for power systems: Tutorial, review, challenges, and prospects. *Electric Power Systems Research*, 223, 109530.
- [14] Makhanov, H., Setia, K., Liu, J., Gomez-Gonzalez, V., & Jenaro-Rabadan, G. (2024). Quantum Computing Applications for Flight Trajectory Optimization. *2024 International Conference on Quantum Communications, Networking, and Computing (QCNC)*, 65-74.
- [15] Ayaz, F., & Nekovee, M. (2024). Quantum Optimization for Bidirectional Telecom Energy Exchange and Vehicular Edge Computing in Green 6G Networks. *2024 IEEE International Conference on Communications, Control, and Computing Technologies for Smart Grids (SmartGridComm)*, 385-390.
- [16] Ho, KTM, Chen, K.C., Lee, L., Burt, F., Yu, S., & Lee, P.H. (2024). Quantum Computing for Climate Resilience and Sustainability Challenges. *2024 IEEE International Conference on Quantum Computing and Engineering (QCE)*, 262-269.
- [17] Munawar, G., & Surendro, K. (2024). Quantum-Based Prediction Model for Carbon Neutrality. *2024 11th International Conference on Advanced Informatics: Concept, Theory and Application (ICAICTA)*.
- [18] Tian, Q., Nie, W., Bao, Q., Niu, W., Li, R., Zhang, X., ... & Akanyange, S. N. (2025). Preparation of red mud derived eggshell coupling adsorbent and study on carbon dioxide capture performance based on experiment and density functional theory simulation. *Separation and Purification Technology*, 355, 129728.
- [19] Morstyn, T., & Wang, X. (2024). Opportunities for quantum computing within net-zero power system optimization. *Joule*, 8(6), 1619-1640.