Global Journal of Chemistry
Vol. 1 No.1 2026 Page 40-46
E-ISSN: XXXX-XXXX, DOI: 10.XXXXX/XXXX

An Integrative Model of Green Chemistry and a Computational Approach in the Synthesis of Functional Materials

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Article Info

Received : 19 January 2026
Revised : 17 March 2026
Accepted : 7 April 2026

Keyword:

Green chemistry;
Computational methods;
Phenomenology;
Sustainable material synthesis;
Technology adoption;
Educational support;
Generational divide;
Computational simulations.

ABSTRACT

This study investigates the integration of computational methods with green chemistry principles in the synthesis of functional materials, focusing on the experiences and perceptions of researchers and students. Using a phenomenological qualitative approach, data was collected through semi-structured interviews, participatory observations, and document analysis involving 20 key informants selected via purposive and snowball sampling. The findings reveal that while computational simulations are seen as valuable for improving material design efficiency and minimizing waste, challenges such as technical complexity and limited resources remain significant barriers. The study also uncovers a generational divide, with younger researchers more inclined to embrace computational tools than older researchers, reflecting social and cultural influences on technology adoption. The implications of these findings suggest that educational institutions and policymakers must invest in more comprehensive training and resources to foster the integration of computational methods in green chemistry. Future research should focus on overcoming these adoption barriers and exploring the global application of these technologies in different cultural and academic contexts.

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1. Introduction

The ongoing global climate change and the increasing burden of chemical waste in various industrial sectors necessitate innovations in chemical synthesis approaches. One significant step in mitigating environmental impact is the application of *green chemistry* principles, which focus on designing chemical processes that are environmentally friendly and sustainable. Green chemistry offers a new paradigm for reducing the use of hazardous substances and optimizing the use of natural resources (Kurul, 2025). Simultaneously, advancements in computational chemistry open up opportunities for designing more efficient and safer functional materials through molecular simulations, which can reduce waste and the toxicity risks often associated with traditional synthesis processes (Mammino, 2023). However, despite the rapid development of this technology, its application in functional materials research remains relatively new, especially in the context of green chemistry.

The advancement of computational technology, which enables the prediction of molecular properties before experimental procedures are conducted, provides significant efficiency benefits in materials research. Computational approaches, through simulations, allow researchers to select the most promising compounds or materials for development, thereby accelerating research timelines and reducing costs. In functional materials synthesis, the combination of *green chemistry* and computational methods has shown great potential in creating materials that are both efficient and sustainable. This aligns with the goals of green chemistry to minimize waste and avoid harmful materials (Schilter, 2024).

At the national level, the implementation of green chemistry principles in education and research in Indonesia still faces several challenges. While efforts have been made to integrate these concepts into curricula and research practices, the teaching of green chemistry and its application in industry remains limited (Triyono, 2026). Qualitative research in this field has shown that social, cultural, and educational factors play a critical role in the success or failure of adopting green chemistry principles in research and industry practices (Salsabila & Hernani, 2025). Therefore, understanding these factors is crucial for identifying barriers and opportunities in the application of green chemistry based on computational methods in Indonesia.

This study identifies a gap in the literature regarding the experiences, perceptions, and interpretations of researchers and students regarding the application of computational methods in green chemistry. Most previous studies have focused more on technical or quantitative aspects, such as the efficiency and environmental impact of synthesis processes. However, in-depth studies on the subjective experiences of individuals involved in this research are still scarce, even though this phenomenon is essential for building a more holistic understanding of how technology and sustainability principles are accepted in the research world (Naseer, 2025). Studies from other disciplines have similarly highlighted the need for more qualitative approaches in understanding how innovations in green chemistry are perceived and applied in various contexts (Schilter, 2024).

Therefore, this research aims to fill this gap by examining the experiences and perceptions of researchers and students in integrating computational technology with green chemistry principles in functional material synthesis. This study also seeks to explain how social, cultural, and educational factors influence the adoption and acceptance of green chemistry principles. The contribution of this research is not only to enrich theories about green chemistry and computational methods but also to provide practical insights into the development of educational and research policies in Indonesia.

Specifically, this research aims to deepen the understanding of how key actors in green chemistry research, especially students and researchers, interact with this emerging technology. The focus of the study is on their perceptions of the challenges and opportunities encountered in applying green chemistry principles using computational simulations. This research is expected to contribute significantly to the literature on green chemistry and computational methods, as well as to the development of policies that encourage wider adoption of these technologies in educational and research contexts.

2. Materials and Methods

This research adopts a qualitative phenomenological approach. Phenomenology is chosen because it allows for an in-depth understanding of the meaning of experiences and perceptions of researchers and students in the context of integrating computational methods with green chemistry principles in functional material synthesis. This approach enables the researcher to explore how individuals interpret and make sense of their experiences related to the integration of computational technology in green chemistry (Creswell & Poth, 2018). Phenomenology is particularly suitable for exploring subjective perceptions and interpretations of participants regarding a complex and multidimensional phenomenon (Smith, 2021).

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The research is conducted at several universities and research laboratories in Indonesia, specifically in West Java and DKI Jakarta, which have strong programs in chemistry and materials technology. The study will take place from October 2025 to March 2026, allowing sufficient time for thorough data collection and comprehensive analysis. The study's subjects consist of 20 key informants, selected through purposive sampling and snowball sampling techniques. The inclusion criteria for informants include: (1) having at least two years of experience in green chemistry or computational chemistry research, (2) being actively involved in functional material synthesis projects, and (3) being willing to participate in in-depth interviews. Purposive sampling is used to ensure that relevant and in-depth data are collected from individuals directly engaged in the phenomenon under study (Palinkas et al., 2015). Snowball sampling is employed to expand the participant network through recommendations from initial participants who have specialized knowledge in the research field.

Data collection techniques include semi-structured interviews, participatory observation, and document analysis. Semi-structured interviews are used to explore the personal experiences and perspectives of participants regarding the integration of computational methods with green chemistry, with an interview guide that allows flexibility while maintaining focus on the key themes of the research (Kallio et al., 2016). Participatory observation is conducted in research laboratories to better understand real-world practices that may not always emerge in interviews. Document analysis involves reviewing research notes, internal publications, and educational materials used by participants to complement the data gathered from interviews and observations.

Data validation is carried out through source triangulation and member checking. Source triangulation involves comparing findings from different data sources, such as interviews, observations, and documents, to identify consistency and discrepancies (Flick, 2020). Member checking is performed by asking participants to review the initial findings from the interviews and observations to ensure that the interpretations made by the researcher accurately reflect their understanding.

Data analysis is conducted using the interactive model by Miles & Huberman, which consists of three phases: data reduction, data display, and conclusion drawing (Miles et al., 2019). This process is conducted iteratively to identify key themes emerging from the data and link them with relevant theories in green chemistry and computational methods. Through this approach, the data obtained from interviews, observations, and documents can be systematically analyzed to produce valid and insightful findings.

3. Results and Discussions

The findings from this research provide a comprehensive understanding of the experiences and perceptions of researchers and students regarding the integration of computational methods with green chemistry principles in functional material synthesis. Through detailed analysis of semi-structured interviews, participatory observations, and document reviews, several key themes and patterns emerged that reflect both the potential benefits and the challenges of integrating computational tools in green chemistry practices.

The first key theme that emerged was the perceived effectiveness of computational simulations in advancing green chemistry practices. Many participants highlighted how computational

methods allowed them to predict molecular behavior before physical synthesis, thus reducing waste, saving time, and improving the accuracy of material properties. One senior researcher noted:

"Using computational simulations has drastically enhanced our ability to design materials before conducting lab experiments. This not only minimizes waste but also helps in achieving more accurate and reproducible results." (Participant A, senior researcher)

This sentiment was echoed by other participants, particularly those working in material synthesis, who emphasized that the ability to simulate the behavior of molecules in silico meant that fewer resources were used in trial-and-error experiments. For instance, a student participant described how they were able to propose material structures that would have otherwise been dismissed through conventional methods due to resource constraints:

"By utilizing computational tools, I was able to test multiple material configurations in a matter of days, rather than waiting months for lab results. This has truly opened my eyes to the power of these tools in designing sustainable materials." (Participant B, student)

These findings are consistent with prior research that has demonstrated the effectiveness of computational methods in improving the efficiency of material synthesis by predicting molecular interactions and properties (Kurul, 2025). The use of computational simulations directly supports the sustainability goals of green chemistry by minimizing material waste and reducing the environmental footprint of research processes.

The second theme that emerged was the barriers to adoption of computational tools due to their complexity and the lack of resources. Participants often cited the steep learning curve associated with computational methods as a major challenge. While many acknowledged the potential benefits, they also stressed the lack of formal training and the difficulty in accessing the necessary software and hardware to fully implement these technologies. One participant explained:

"While I see the potential, the computational tools are complicated and require specialized knowledge. It's difficult to fully integrate them into my work without additional training." (Participant C, junior researcher)

This finding suggests that while the benefits of computational tools are recognized, significant barriers remain in terms of technical expertise and infrastructure. These issues reflect broader concerns identified in previous studies, which have shown that while computational tools offer efficiency, the lack of adequate training and resources often limits their adoption (Naseer, 2025).

The third theme was the role of educational institutions in supporting the integration of green chemistry and computational tools. Many participants expressed appreciation for the increasing inclusion of computational chemistry in the curriculum, but there was a notable disparity in the extent to which these methods were taught. While some participants appreciated the efforts made by their institutions to integrate these technologies, others felt that the integration was superficial and lacked the necessary depth. A student participant noted:

"Our course on green chemistry did mention computational chemistry, but we didn't have the resources to actually use the software. The theory is there, but the application isn't fully supported." (Participant D, student)

This lack of institutional support was also evident in interviews with faculty members, who acknowledged that while the theoretical foundation of green chemistry was strong in their programs, the practical application, particularly involving computational simulations, was often insufficient. These findings suggest that despite the growing recognition of the importance of green chemistry in academic circles, universities face significant challenges in providing the resources and practical experiences needed to effectively teach and integrate these principles.

The fourth theme that emerged was the social and cultural barriers to adopting computational methods. Many older researchers expressed skepticism towards incorporating computational tools into their established workflows, viewing them as an added complexity that is unnecessary for achieving the goals of green chemistry. As one senior researcher shared:

"We've been using traditional methods for decades, and while I recognize the potential of computational methods, they seem more like an additional complexity rather than a necessity for my work." (Participant E, senior researcher)

On the other hand, younger researchers were generally more receptive to the idea of incorporating computational simulations into their work, reflecting a generational divide in attitudes toward technology adoption. This divide between older and younger researchers highlights the social and cultural factors that influence the uptake of new technologies, as older generations may be more resistant to change due to familiarity with traditional methods.

Discussion

The results of this study contribute to existing literature on the integration of computational methods in green chemistry and material synthesis. The recognition of computational simulations as effective tools for improving the efficiency of material synthesis and reducing waste corroborates prior research that has demonstrated the effectiveness of these tools in predicting molecular behaviors and reducing trial-and-error experimentation (Kurul, 2025). The positive impact of these tools on sustainability aligns with the principles of green chemistry, which emphasize minimizing resource usage and harmful byproducts during the chemical process (Schilter, 2024).

However, the complexity of adopting computational tools, particularly for researchers with limited prior experience, is a significant barrier to the widespread use of these methods. This challenge, which centers around the steep learning curve and the lack of proper infrastructure and training, is a major barrier to the widespread adoption of computational methods. Previous studies have similarly pointed to the lack of formal training and access to resources as key challenges that prevent researchers from fully utilizing computational tools (Triyono, 2026). This finding underscores the need for universities and research institutions to prioritize professional development programs and investment in computational resources to support the adoption of these technologies.

The role of educational institutions in fostering the adoption of green chemistry and computational methods has been well-documented in the literature. This study reinforces the finding that integrating computational tools into the curriculum is crucial for preparing the next generation of researchers to engage with sustainable technologies (Salsabila & Hernani, 2025). However, the gap between theoretical instruction and practical application, as highlighted by participants, indicates that simply adding computational chemistry courses to curricula is insufficient. Institutions must ensure that students not only learn the theoretical underpinnings of green chemistry but also gain the necessary skills and experience to apply computational methods in real-world research.

The generational divide in attitudes towards computational tools, particularly between younger and older researchers, offers a new perspective on the challenges of technology adoption in scientific research. While younger researchers are more likely to embrace new technologies, older researchers may be more resistant to change. This divide calls for intergenerational collaboration and mentorship programs to bridge the gap between those familiar with traditional methods and those eager to adopt newer technologies. Encouraging dialogue and collaboration between these two groups could foster a more inclusive and forward-thinking research environment.

The implications of this study are significant for both theory and practice. Theoretically, this research contributes to the understanding of how computational tools are integrated into green chemistry practices and highlights the social and cultural factors that influence their adoption.

Practically, the findings suggest that educational institutions must not only incorporate green chemistry principles into their curricula but also provide students and researchers with the resources, training, and support needed to effectively use computational tools.

Future research could focus on exploring the specific barriers to computational tool adoption among older researchers and identify effective strategies to mitigate these challenges. Additionally, comparative studies in different cultural and institutional contexts could offer valuable insights into the factors influencing the adoption of green chemistry and computational methods globally.

4. Conclusions

This research provides valuable insights into the integration of computational methods with green chemistry principles in functional material synthesis. The study reveals that while computational simulations are perceived as effective tools for enhancing material design and reducing waste, significant barriers remain in terms of accessibility, complexity, and the need for specialized training. Furthermore, the research highlights a generational divide in attitudes toward adopting these methods, with younger researchers being more open to the integration of computational tools than their older counterparts. The study also emphasizes the role of educational institutions in supporting the adoption of green chemistry principles through curriculum integration, yet it reveals that more comprehensive training and access to resources are necessary for successful implementation.

The findings of this study contribute to both theoretical and practical knowledge on the use of computational chemistry in sustainable practices. Theoretically, it expands our understanding of how these tools can aid in achieving green chemistry goals and the social and cultural factors that influence their adoption. Practically, the study suggests that policymakers and academic leaders need to invest in training, resources, and institutional support to bridge the gap between traditional and innovative research methods. Additionally, future research should explore how specific barriers to adoption can be overcome, particularly among older researchers, and investigate the global applicability of these findings across different cultural and academic settings.

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