Interdisciplinary Integration of Molecular Modeling and Circular Economy for Sustainable Materials and Processes

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Abstract: The integration of Molecular Modeling (MM) and Circular Economy (CE) establishes a scientific basis for designing sustainable materials and optimizing low-impact technological processes. CE provides systemic principles for resource efficiency and material recirculation, while MM offers atomistic and electronic-structure insights that clarify mechanisms essential for circular technological development. Bibliometric data reveal a sharp increase in ECMM studies after 2018, indicating the emergence of a consolidated interdisciplinary field. Case studies demonstrate how MM supports circular strategies by predicting extraction mechanisms in aqueous two-phase systems, evaluating ion selectivity in MOFs, and elucidating adsorption pathways relevant to CO_2 capture and storage. Together, these applications show that MM enhances process predictability, reduces experimental demand, and accelerates the development of regenerative, carbon-efficient technologies aligned with CE principles. This convergence, therefore, strengthens the scientific foundation necessary for scalable circular solutions and contributes to global decarbonization efforts.

Keywords: molecular modeling; circular economy; resource recovery; sustainable materials; CO_2 capture.

1. Introduction

Rising global climate change impacts have intensified extreme weather events worldwide, with particularly severe consequences in Brazil. The country's dependence on vulnerable sectors such as agriculture, land use, and hydroelectric generation [1]. Alongside growing pressures on biomes driven by deforestation and persistent emissions, this has reduced ecological resilience and increased national climatic instability. This scenario reinforces the need for mitigation strategies centered on resource efficiency and the valorization of carbon flows.

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In this context, the Circular Economy emerges as a systemic framework that reduces environmental impacts by maintaining materials in continuous production cycles, minimizing waste, and promoting resource regeneration [2]. In parallel, Molecular Modeling has consolidated as a central tool for the development of low-carbon technologies, enabling the prediction of properties, identification of interaction mechanisms, and design of innovative materials for CO_2 capture, transformation, and storage [3-4].

The convergence between CE and MM, therefore, offers an integrated pathway for developing sustainable solutions by combining principles of productive reorganization with atomistic tools capable of optimizing processes and materials. This integration is especially relevant in carbon-mitigation contexts, where molecular-level understanding supports more selective, efficient, and circular technological strategies. To contextualize how this convergence has been approached in the scientific domain, the bibliometric analysis presented below provides a structured overview of the evolution of publications related to CE and MM. This analysis identifies patterns, trends, and emerging areas, positioning the present study within the current scientific landscape and highlighting gaps that inform subsequent case studies.

2. Fundamentals and Scope of the Circular Economy

The Circular Economy constitutes a production and consumption model that prioritizes resource regeneration, waste minimization, and the valorization of materials in closed cycles. Its central objective is to ensure that products and components maintain their functionality and value for extended periods, reducing dependence on primary resources and mitigating environmental impacts in alignment with global carbon-neutrality goals [5- 6].

An illustrative example is the use of fibers from the banana pseudostem, which demonstrates how low-value agricultural residues can be converted into materials with mechanical properties comparable to jute and sisal, enabling the production of hats, bags, and other bio-based artifacts [7]. This reinforces CE's capacity to stimulate innovative solutions, decrease reliance on virgin raw materials, and promote regenerative industrial models aligned with Sustainable Development Goals.

The effectiveness of CE, however, depends on explicit integration across multiple scientific domains, forming an interdisciplinary space that brings together materials science, engineering, sustainability, environmental analysis, and technological innovation. In this context, scientific evaluation, physicochemical characterization, and computational modeling are essential tools for guiding the development of circular products and processes with enhanced accuracy.

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It is at this point that Molecular Modeling plays a strategic role. MM enables the prediction of properties, the optimization of technological routes, and the reduction of experimental steps, thereby strengthening decisions that enhance energy efficiency, waste reduction, environmental mitigation, and sustainable innovation. The articulation between CE and MM thus expands the potential to address global challenges such as resource scarcity, the transition to low-impact materials, and the implementation of production systems consistent with green economy principles.

3. Molecular Modeling as a Tool for Sustainable Innovation

Molecular modeling comprises theoretical and computational methods used to understand the behavior and properties of atoms, molecules, and materials. These tools allow precise prediction of interactions and reduce reliance on resource-intensive experimental procedures [8]. Advances in high-performance hardware and software have significantly expanded its applicability, enabling cost savings, shorter development timelines, and optimized laboratory workflows [9].

An emblematic example of this advancement can be seen in recent initiatives that employ high-performance chemical simulations to investigate per- and polyfluoroalkyl substances (PFAS). PFAS are persistent organofluoride compounds known for their extreme molecular stability, resistance to biodegradation, and ability to bioaccumulate, posing global environmental and health challenges [10].

Given their persistence and hazardous profile, the search for efficient remediation pathways for PFAS contamination has become an international priority. In this context, MM accelerates investigations into degradation mechanisms, particularly defluorination, the rupture of carbon–fluorine bonds, which are among the strongest in chemistry. Understanding these processes computationally enables the design of remediation strategies with reduced experimental dependence, contributing to material circularity and reducing chemical pollution within CE frameworks.

4. Scientific Trends in the Convergence of Molecular Modeling and Circular Economy

Bibliometric analysis of the Scopus database highlights trends in publications on Molecular Modeling, the Circular Economy, and their intersection. For this purpose, predefined keywords were used as search criteria: for MM, the set “molecular AND (modeling OR modelling OR simulation)” was employed; for CE, “circular AND economy” was

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adopted; and to identify studies that simultaneously integrate both fields, the combination "circular AND economy AND molecular AND (modeling OR modelling OR simulation)" was used. The bibliometric trends presented in Figure 1 contextualize the scientific evolution of the ECMM field, guided the collection and organization of data over the past two decades, and enable a temporal visualization of scientific advancements in these fronts.

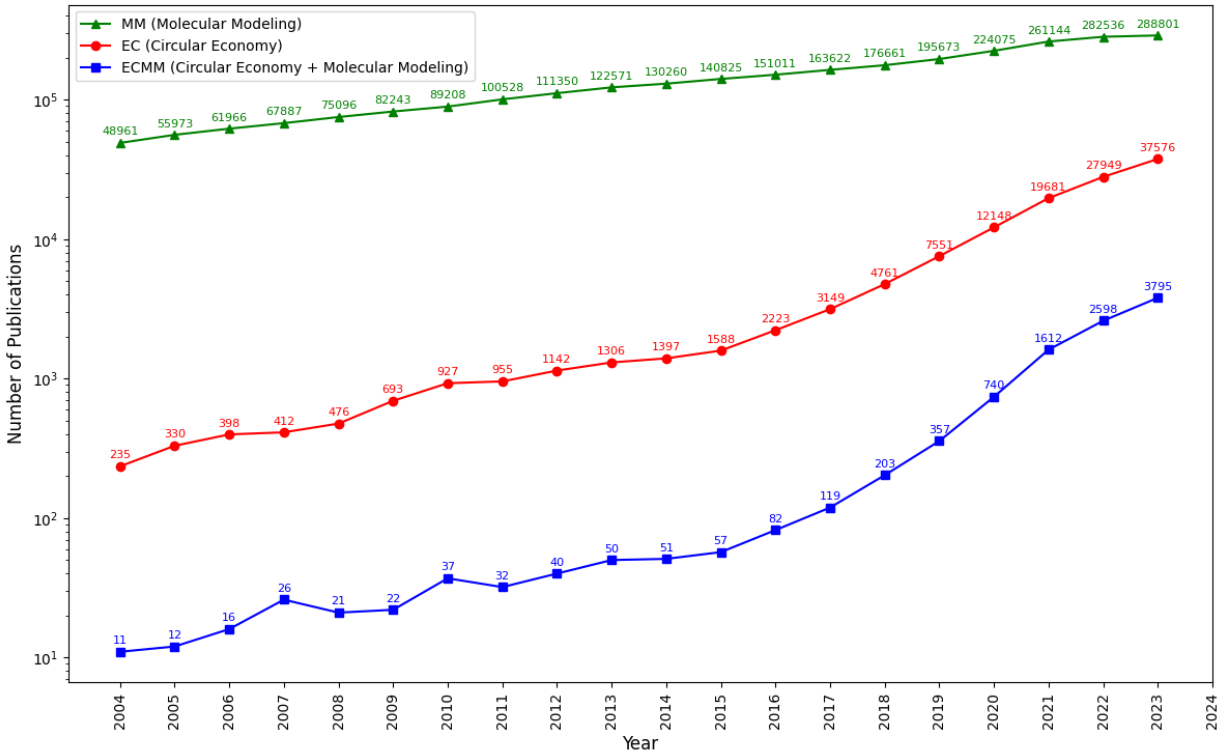

Figure 1. Temporal evolution of publications in the MM, CE, and ECMM categories (2004- 2024).

The observed pattern demonstrates that the most significant trend is the sharp post-2018 increase in publications combining MM and CE. This growth reveals the consolidation of an explicitly interdisciplinary approach, in which MM is no longer restricted to theoretical chemistry and has become part of a methodological repertoire applied to sustainability, materials science, process engineering, sustainable mining, and technological innovation. The rise of the ECMM category indicates that researchers recognize the strategic role of computational modeling for circular processes, the recovery and recycling of critical materials, the development of low-impact pathways, and the creation of clean technologies capable of both reducing emissions and minimizing waste.

This bibliographic evolution reaffirms the potential of ECMM integration as a scientific instrument for addressing global environmental challenges widely debated in international documents, such as those discussed at COP30 in 2025. The observed trends

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align with central themes related to the integration of economy, environment, and technology, especially in the context of the transition to a green economy, the productive transformation toward circular systems, and the role of digital innovations in mitigating environmental impacts [11]. Thus, the continuous growth of ECMM publications demonstrates that the interface between computational chemistry and circularity not only constitutes an emerging research front but also forms a structuring axis for the development of scientific solutions capable of addressing, in an integrated manner, resource scarcity, and the need for new sustainable production frameworks.

5. Computational Solutions to Contemporary Circular Economy Challenges

The integration of MM and CE enables multidisciplinary approaches that can transform production practices and accelerate the transition to sustainable models. Challenges such as critical-metal recovery, catalyst development, solvent optimization, and alternative recycling pathways can be investigated with high precision through simulations, reducing experimentation, emissions, and costs.

In industrial applications, particularly in mineral extraction, MM contributes to the optimization of separation processes. The calculations elucidated mechanisms in aqueous two-phase systems (ATPS), which are proposed as eco-friendly alternatives for extracting Co(II), Ni(II), and Fe(III). These systems, formed by polyethylene oxide and thiocyanate salts, enable selective and energy-efficient extraction. The results elucidate stabilization mechanisms, binding affinities, and selectivity patterns. This understanding supports the development of more regenerative and efficient routes, decreasing experimental steps, energy demand, and waste generation, in alignment with CE principles [12].

Another relevant application involves investigating the selectivity of porous materials, such as the Metal Organic Framework (MOF) UiO-66, used in ionic separation processes. Density Functional Theory (DFT) calculations and short-term experiments have revealed how structural and electronic features affect hydrated cation transport, informing strategies for recovering high-value metals like lithium. Predictive modeling reduces repetitive experimentation and fosters circular production chains by recirculating critical materials [13].

Regarding CO_2 capture, reuse, and storage, which are essential for addressing the impacts of climate change, atomistic simulations allow detailed evaluation of the structural, energetic, and electronic properties of materials. These insights provide a basis for optimizing adsorbent surfaces and clarifying interaction mechanisms before experimental testing. This demonstrates how MM supports transitions from linear to circular production models by guiding the development of low-carbon technologies.

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The effectiveness of this approach has been demonstrated in different studies. Investigations into interactions between CO_2 and asphaltene models using DFT calculations reveal that the presence of heteroatoms modulates aromatic aggregation and alters the stability of dimers under conditions relevant to CO_2 reinjection in reservoirs [14]. These results are significant for geological sequestration, as structural variations at the molecular level influence macroscopic oil properties (such as viscosity, mobility, and flow behavior), allowing better anticipation of trapping efficiency and long-term reservoir stability. This molecular-level perspective improves the predictability and safety of geological storage operations, contributing to the development of more effective mitigation technologies aligned with global emission reduction goals.

Complementing this perspective, investigations into nitrogen-doped carbon materials demonstrate how substitution patterns modulate electrostatic potentials and surface reactivity, affecting CO_2 adsorption pathways. These predictions support the rational design of more selective and energetically favorable adsorbents, strengthening circular and climate mitigation technologies [15]. Understanding these effects at the molecular scale reinforces the predictability and efficiency of CO_2 capture technologies, contributing to strategies aligned with circular economy principles and climate change mitigation.

6. Conclusions

The integration of the Circular Economy and Molecular Modeling emerges as a promising strategy for climate change mitigation by combining the regenerative reorganization of production systems with the design of materials and processes capable of capturing, transforming, and storing CO_2. The case studies demonstrate that MM elucidates, at the molecular level, factors that contribute to the affinity and stability of low-carbon systems, guiding the development of solutions compatible with CE principles. Future advances include expanding multiscale models, applying machine-learning techniques, and the application of MM in hybrid systems for sustainable CO_2 capture and conversion. This thereby strengthens the synergy between CE and MM and contributes to more efficient technologies aligned with global decarbonization targets.

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