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Evaluating Norbornadiene/Quadricyclane for Solar Thermal Energy Storage: A Systematic Review Using Methodi Ordinatio

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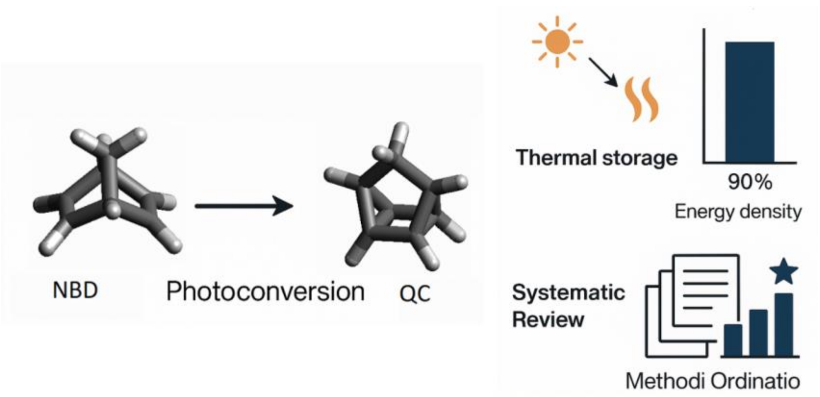
This work presents a comprehensive systematic review of the potential of Norbornadiene/Quadricyclane (NBD/QC) as a promising molecular system for solar thermal energy storage (MOST). Utilizing the Methodi Ordinatio methodology, this study aims to identify, classify, and rank the most impactful research articles based on a weighted combination of their citation count, impact factor, and year of publication. A complete literature search was performed across the Scopus, ScienceDirect, and Web of Science databases using targeted keywords such as "Norbornadiene," "Quadricyclane," and "solar thermal energy storage." A complete literature search across Scopus, ScienceDirect, and Web of Science using targeted keywords initially identified 567 studies; after applying relevance criteria, 341 articles published between 2014 and 2024 were selected for detailed analysis. The saved studies were then ranked using the InOrdinatio index, ensuring a data-driven prioritization of the most relevant contributions to the field. The analysis highlights recent technological advancements in NBD/QC-based solar energy systems, focusing on photoconversion efficiencies exceeding 90%, energy densities reaching up to 966 kJ/kg, improvements in isomerization kinetics, and enhanced thermodynamic stability of their metastable states. This systematic review not only contributes to the growing body of knowledge on molecular solar thermal systems but also offers strategic reflections for advancing sustainable and efficient solar energy technologies.

Graphical abstract



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1. Introduction

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The growing demand for sustainable energy solutions is driving the development of innovative technologies for capturing, storing, and utilizing renewable energy. Among these technologies, Molecular Solar Thermal Energy Storage (MOST) systems stand out for offering a promising approach to harnessing solar energy [1]. Unlike traditional thermal storage systems, MOST uses photosensitive molecules that capture and store solar energy in the form of chemical energy, which can later be released as heat on demand. This technology has the potential to address the challenges of solar intermittency, enabling continuous use of captured energy even in the absence of sunlight [2]. Despite notable advances, a systematic prioritization of the most impactful studies on MOST technologies remains limited, particularly concerning the NBD/QC system.

One of the most studied molecular pairs for MOST systems is Norbornadiene/Quadricyclane (NBD/QC). The NBD/QC pair consists of molecules that, when exposed to sunlight, undergo photochemical isomerization, converting Norbornadiene (NBD) into Quadricyclane (QC). During this transformation, solar energy is stored in high-energy chemical bonds. The stored energy can be released in a controlled manner through the thermal or catalytic reversion of QC back to NBD, releasing heat for potential applications in power generation or heating [3].

The NBD/QC pair offers several advantages: in addition to providing high energy density and photochemical reversibility, the system eliminates the need for traditional batteries since the storage occurs purely at the molecular level. Thus, it becomes highly promising for applications in regions with high solar incidence, allowing solar energy to be stored during periods of high capture and used during low irradiance times, such as at night or on cloudy days. Furthermore, the chemically controlled process offers greater flexibility in utilizing the stored energy [4,5]. However, a comprehensive, data-driven evaluation of NBD/QC's scientific progress is essential to guide future innovations and overcome persisting limitations.

Nevertheless, significant challenges remain in enabling the widespread application of NBD/QC in MOST systems. One of the main obstacles is optimizing the thermal stability of the molecules over multiple isomerization and reversion cycles, as molecular degradation can reduce system efficiency over time. Another challenge is improving energy conversion efficiency and developing catalysts that can accelerate energy release without compromising the system's integrity. These issues make research in this area crucial for advancing energy storage technologies [6]. Despite previous reviews on MOST systems, a systematic, data-driven prioritization of NBD/QC studies is still lacking, which this work aims to address.

To identify the most relevant contributions and the state of the art in this field, this study uses the Methodi Ordinatio methodology to conduct a systematic literature review on the NBD/QC pair as an ideal candidate for MOST systems [7]. Methodi Ordinatio is an approach that allows the classification and organization of scientific articles based on three main factors: journal impact, citation count, and publication year, ensuring that the most relevant and current studies are prioritized [8]. This work aims to provide a detailed overview of the advances in the field, identify knowledge gaps, and suggest directions for future research that may help overcome the challenges in developing MOST systems based on NBD/QC.

2. Material and Methods

All procedures were conducted following the Methodi Ordinatio methodology, which comprises nine structured phases: (i) defining the research topic, (ii) selecting relevant keywords, (iii) searching academic databases, (iv) filtering initial results, (v) identifying key terms and themes, (vi) eliminating duplicates, (vii) systematically reading abstracts and full texts, (viii) critical evaluation, and (ix) final article selection and ranking [7]. This approach was adapted from the ProKnow-C method, which emphasizes a systematic and objective portfolio construction process based on bibliometric indicators.

The literature search was performed across four major academic databases—ScienceDirect, Web of Science, Scopus, and Google Scholar—chosen due to their broad coverage, multidisciplinary reach, and relevance to the fields of materials science and renewable energy. The InOrdinatio index was applied to rank the articles based on three main criteria: year of publication, journal impact factor (or alternative journal metrics where applicable), and citation count. This ranking ensures that the most relevant and high-impact studies on NBD and QC for solar thermal energy storage are prioritized [7].

To refine the portfolio, Mendeley reference manager software was used to remove duplicate entries and irrelevant articles. Furthermore, this work incorporated the updated Methodi Ordinatio 2.0 methodology, which introduced statistical enhancements and automated tools such as FInder and RankIn. These tools significantly improved data collection, portfolio construction, and the overall accuracy and reproducibility of the ranking process [8].

3. Results and Discussion

3.1. Bibliometric Trends and Publication Highlights

A total of 567 articles were initially retrieved from the database searches. Following duplicate removal and the exclusion of studies whose titles and abstracts were not aligned with the research topic, a refined portfolio of 341 relevant articles was established.

Figure 1 illustrates the distribution of publications related to NBD/QC systems for solar thermal energy storage over the past decade.

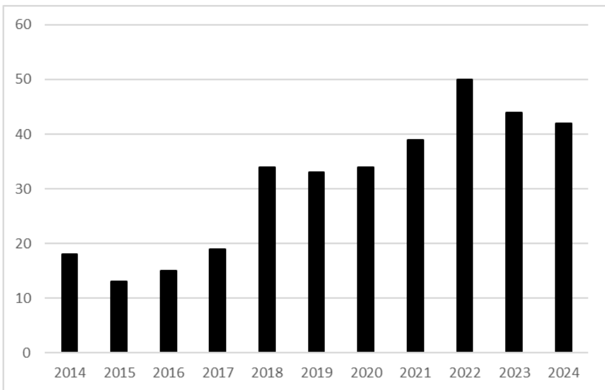

Fig. 1. Number of published articles in the field studied in the last decade.

The data indicate a steadily growing scientific interest in molecular solar thermal (MOST) energy storage systems, particularly after 2018. A notable peak of 50 articles published in 2022 reflects increased research efforts, likely driven by the urgent demand for sustainable energy alternatives and the advancement of photomolecular storage technologies.

The slight fluctuation in publication numbers observed after 2020 may reflect the compounded effects of the COVID-19 pandemic on global research activities, including decreased laboratory productivity and redirected research funding towards health-related priorities [9]. Nevertheless, despite a modest decline to 44 articles in 2023 and 42 in 2024, the field remains vibrant and dynamic, suggesting that the NBD/QC system continues to attract considerable scientific and technological interest for solar energy storage applications.

Overall, the consistent research output highlights a sustained interest in enhancing MOST systems through hybrid materials, molecular engineering, and nanostructuring approaches. The highest-ranked article according to the InOrdinatio index was authored by Wang et al. (2021). This study proposed the integration of NBD molecules with nanomaterials and the application of steric strain to enhance energy storage capacity, representing a significant advancement towards the development of more efficient solar thermal fuels [10]. Table 1 presents the top 10 articles ranked according to the InOrdinatio index, illustrating the most influential studies on the NBD/QC system for MOST applications.

Table 1. Top 10 articles on the NBD/QC system for MOST applications ranked by the InOrdinatio index.

Ranking	Author	Number of citations	Periodic Impact factor	InOrdinatio index
1	(Wang et al., 2021)	105	50.1	254.510
2	(Wang et al., 2019)	134	54	250.017
3	(Dreos et al., 2017)	111	54	215.657
4	(Kashyap et al., 2019)	78	50.1	200.984
5	(Orrego-Hernández et al., 2020)	114	36.1	198.447
6	(Zhang et al., 2018)	265	7.5	172.349
7	(Mansø et al., 2018)	117	23.2	134.878
8	(Sun et al., 2019)	116	6.2	94.617
9	(Lennartson et al., 2015)	190	4.3	86.531
10	(Quant et al., 2016)	109	9.1	73.639

Note: The InOrdinatio index was calculated based on citation number, impact factor, and publication year, following the methodology proposed by Pagani et al. (2015) [7].

The second-ranked article by Wang et al., published in 2019, centers on optimizing heat release in MOST systems, a key factor for practical energy storage applications [11]. Among the key studies, Dreos et al. (2017) showcase NBD's notable energy density (up to 966 kJ/kg) and stability, presenting it as superior to lithium-ion batteries and phase-change materials (PCMs), especially for remote applications like satellite thermal control [12]. The study by Kashyap et al. (2019) introduced a hybrid system that combines NBD/QC molecular storage with phase-change materials, enabling full-spectrum solar energy harvesting and storage. This system achieved remarkable efficiencies of up to 90% during the day and 80% at night, along with high material stability [13].

Building upon these advancements, Orrego-Hernández et al. (2020) further optimized NBD/QC systems specifically for solar thermal storage, attaining an improved match with the solar spectrum, a high energy density of up to 0.9 MJ/kg, and tunable storage stability [14]. In a subsequent investigation, Zhang et al. (2018) underscore the high potential of NBD and its isomer QC for high-energy density applications, pointing out that with advances in synthesis and reduced costs, these compounds could become key components for sustainable and efficient fuels [15].

Subsequently, Mansø et al.'s 2018 study presents advanced synthetic protocols for NBD dimers and trimers, achieving high photoconversion yields of up to 94% and energy densities up to 927 kJ/kg, well beyond the target of 300 kJ/kg, positioning NBD as a promising candidate for thermal energy storage [16]. Sun et al. (2019) reinforce NBD's potential, focusing on cobalt-phthalocyanine (CoPc)-catalyzed isomerization of QC to NBD [17].

The work by Lennartson et al. (2015) highlights the critical importance of designing durable photoswitches for molecular solar thermal (MOST) systems, emphasizing the development of molecules capable of efficiently storing energy, maintaining thermal stability, and withstanding multiple switching cycles—factors that are essential for the successful application of NBD/QC in MOST technologies [18]. In a similar context, the study by Quant et al. (2016) proposes that hybrid systems combining solar water heating with MOST technologies could significantly enhance energy storage efficiency, further supporting the integration of NBD/QC as a promising approach [19].

Together, these studies reveal a consistent trend towards hybridization and nanostructuring as strategies to enhance energy density and stability in NBD/QC systems. To support the understanding of the NBD/QC cycle and its mechanism for solar thermal energy storage, a schematic representation is provided in Figure 2.

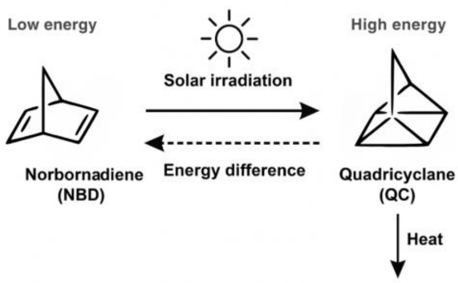

Fig. 2. Schematic representation of the Norbornadiene/Quadricyclane (NBD/QC) system for solar thermal energy storage. Solar irradiation induces the conversion of NBD into the high-energy QC isomer, which can revert thermally or catalytically to release stored heat.

3.2. Technological Applications Beyond Energy Storage

Beyond its primary use in solar thermal energy storage, the NBD/QC system has shown promise for other technological applications. Recent studies have suggested that these photoresponsive molecules could be integrated into photomechanical actuators, smart windows, and responsive coatings due to their reversible isomerization and ability to release heat on demand [17]. Additionally, the QC isomer's higher energy content and structural rigidity have made it a candidate for temporary mechanical energy storage and release in micro-electromechanical systems (MEMS) [20]. These emerging applications suggest a broader technological potential for the NBD/QC pair, further motivating continued research into its optimization and integration into multifunctional devices.

3.3. Challenges and Limitations of the NBD/QC System

Despite the promising performance of NBD/QC-based MOST systems, several critical challenges must be addressed to enable their widespread implementation. A primary concern is the thermal and photochemical stability of the QC isomer during long-term storage, as degradation over time can severely impact efficiency. Additionally, many derivatives of NBD still exhibit low quantum yields or poor absorption in the visible range, limiting their practical use under natural sunlight [14]. Another important barrier is the scalability of synthesis most high-performance NBD derivatives require multi-step synthetic routes involving expensive reagents or complex purification steps [15]. Finally, ensuring reversible and efficient isomerization over multiple charge/discharge cycles without catalyst deactivation or byproduct formation remains a technological bottleneck. These limitations underscore the need for continued innovation in molecular design, material integration, and catalytic strategies.

4. Conclusions

This study utilized the Methodi Ordinatio methodology to systematically classify and rank the most relevant articles on the Norbornadiene/Quadricyclane (NBD/QC) system for Molecular Solar Thermal Energy Storage (MOST). The results offer a detailed overview of the scientific advancements in the field, highlighting key contributions that address energy density, photochemical reversibility, and thermal stability.

By focusing on the most recent and highly cited studies, this work provides a solid foundation for future research. In addition to its potential for MOST applications, recent findings also indicate that the NBD/QC system may serve as a versatile platform for other technological uses, including smart coatings, photomechanical actuators, and energy-release microdevices such as MEMS. These emerging applications further expand the relevance of this molecular pair in the context of renewable and responsive materials.

Despite the progress made in understanding and optimizing the NBD/QC system, challenges such as molecular degradation, low quantum yields, poor visible light absorption, and the complexity of synthesis remain critical barriers to large-scale adoption. The relatively small number of focused studies in this area, as revealed by this review, underscores the need for continued research to refine the stability, efficiency, and scalability of these systems.

Future investigations should prioritize overcoming these obstacles by exploring novel catalytic processes, enhancing molecular resilience across multiple storage and release cycles, and developing hybrid systems that integrate MOST with other renewable or multifunctional technologies. By addressing these gaps, the NBD/QC system could play a crucial role in advancing sustainable solar energy storage and other smart energy applications.

These findings suggest that, with sustained interdisciplinary research, NBD/QC-based systems may become integral components of future energy infrastructures supporting applications that range from satellite thermal regulation and residential energy storage to photomechanical control in smart devices.

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Author Contributions

Roberto Ribeiro Faria: Conceptualization, Methodology, Formal analysis, Investigation, Validation, Resources, Writing – Original Draft. Fernando Freitas Siqueira Silva: Data Curation, Writing – Review & Editing. Odonírio Abrahão Júnior: Supervision, Project administration, Funding acquisition, Writing – Review & Editing.

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