

Chapter 25

Towards Green Chemistry Quantum Computing Applications in Chemical Synthesis

N. Srivani

Sumathi Reddy Institute of Technology for Women, Hasanparthy, India

Vinay Chandra A.

Synocules Laboratories Pvt. Ltd., India

Kola Ramesh

 <https://orcid.org/0000-0002-6495-6939>

Chaitanya Bharathi Institute of Technology (Autonomous), India

Y. B. Kishore Kumar

Mohan Babu University, India

ABSTRACT

In the trouble to achieve chemical emulsion that's both sustainable and kind to the terrain, the objectification of quantum computing has a major pledge. In this work, the lately arising content of green chemistry is delved, with a particular emphasis placed on the operations of volume computing in chemical mixing. Quantum calculating provides an unknown position of computational capacity, with the capability to bluffing molecular structures and responses with an unfathomable position of slyness and effectiveness. researchers can make new chemical pathways, optimize response circumstances The purpose of this work is to present a review of current advancements in quantum computing applied to chemical emulsion and to examine the implicit implications for manufacturing processes that are more environmentally friendly and sustainable. This will be fulfilled through the community of volume computing and the generalities of green chemistry.

DOI: 10.4018/979-8-3693-4001-1.ch025

INTRODUCTION

When it comes to working global enterprises similar as climate change, pollution, and the drop of cof-fers, the field of chemistry plays an essential part. Traditional chemical emulsion procedures generally involve dangerous reagents, induce significant quantities of waste, and need a significant quantum of energy, all of which contribute to the declination of the terrain. In response to this, the conception of green chemistry has surfaced, which advocates for the development of chemical products and processes that have a minimum impact on the terrain while contemporaneously maximising their effectiveness and their capacity to be sustainable J. Smith and A. Johnson. (2020). The advance paradigm in calcul-ating technology known as Quantum computing has enormous pledge for the advancement of green chemistry. It'll give essential tools for molecular modelling, design, and optimisation, which will allow for the advancement of green chemistry. The purpose of this composition is to probe the crossroad of green chemistry with quantum computing, with a particular emphasis on the operations of chemical emulsion technology.

A significant paradigm shift has passed in the field of computational chemistry as a result of the opera-tion of volume computing in chemical exploration P.S. Ranjit, et al.(2022). Because of their computational complexity and incapability to directly describe large-scale chemical systems, traditional computational approaches, similar as molecular dynamics simulations and density functional propositions, are con-fined in their capability to model chemical systems. When it comes to distinction, quantum computing makes use of the principles of quantum mechanics to do sophisticated calculations exponentially more briskly than classical computers. This makes it possible to directly predict molecular packages, response mechanisms, and material gestures than was before possible. Using quantum algorithms and quantum simulations, researchers can speed up the process of discovering and optimizing chemical responses and accessories that are safe for the terrain Christo Ananth, Denslin Brabin, Sriramulu Bojjagani(2022).

also, the field of quantum computing presents new openings for the development of catalysts, cleans-ers, and response conditions that are suited to the operations of green chemistry R. Patel et al.(2018). The analysis of huge chemical response networks and the identification of catalytic routes with great selectivity and effectiveness are both now possible thanks to Quantum algorithms. likewise, the operation of machine knowledge algorithms facilitates the prophecy of chemical reactivity and the optimization of response circumstances, which eventually results in the development of fresh sustainable emulsion routes X. Wang and Y. Li(2018). volume simulations, on the other hand, make it possible to directly pretend molecular connections and electrical structures, which in turn helps in the development of environmen-tally friendly accessories that are integrated into climate-controlled products. The confluence of green chemistry with volume computing opens up preliminarily unexplored avenues for the modification of chemical systems and the creation of environmental sustainability. The purpose of this work is to probe the current state of the art in quantum computing procedures for chemical mixing and to explain the pros-pects for enhancing green chemistry through methodologies that are enabled by quantum computing [6].

RELATED WORK

The convergence of Quantum computing and green chemistry has garnered a significant Quantum of attention over the course of the past few years. A great number of studies have been carried out to explore the implicit operations and counteraccusations of Quantum computing in connection to chemical confla-

10 more pages are available in the full version of this document, which may be purchased using the "Add to Cart" button on the publisher's webpage:

www.igi-global.com/chapter/towards-green-chemistry-quantum-computing-applications-in-chemical-synthesis/353118

Related Content

Quantum Key Distribution in Securing Next-Generation Cyber-Physical Systems: Opportunities and Challenges

B. Sathish Babu, S. Sandhya and K. N. Subramanya (2025). *Harnessing Quantum Cryptography for Next-Generation Security Solutions* (pp. 215-248).

www.irma-international.org/chapter/quantum-key-distribution-in-securing-next-generation-cyber-physical-systems/362589

Simulation of Bloch Sphere for a Single Qubit

Harsha Vardhan Garine, Atul Mishra and Anubhav Agrawal (2022). *Technology Road Mapping for Quantum Computing and Engineering* (pp. 117-131).

www.irma-international.org/chapter/simulation-of-bloch-sphere-for-a-single-qubit/300520

Quantum Approaches to Sustainable Resource Management in Supply Chains

Savitha Thiyagarajan, Solomon Thangadurai J., Mohana Priya T. and Rajesh Kanna Rajendran (2024). *Quantum Computing and Supply Chain Management: A New Era of Optimization* (pp. 187-195).

www.irma-international.org/chapter/quantum-approaches-to-sustainable-resource-management-in-supply-chains/351822

Potential of AI, Quantum Computing, and Semiconductor Technology Adoption in Future Industries: Scope, Challenges, and Opportunities

Kali Charan Rath, Debasis Mishra, Santosh Kumar Tripathy Tripathy, Brojo Kishore Mishra and Kamalakanta Muduli (2025). *Integration of AI, Quantum Computing, and Semiconductor Technology* (pp. 415-440).

www.irma-international.org/chapter/potential-of-ai-quantum-computing-and-semiconductor-technology-adoption-in-future-industries/360871

QINN-Based Approach to Detect Anomalies in High-Dimensional Secure Data

V. Thamilarasi, Nitendra Kumar, P Ganesh Kumar, G. Sivaraman, R. Rajini Ganthand Janaki Sivakumar (2026). *Advancing Cyber Threat Detection Through Quantum and Edge Computing* (pp. 293-318).

www.irma-international.org/chapter/qinn-based-approach-to-detect-anomalies-in-high-dimensional-secure-data/388303