Impact of Information Technology in Chemical Research

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Abstract

The field of Information Technology has developed vastly in a past few decades and is used as an integral part of advanced research in many areas. Information technology provided chemical science and technology with truly remarkable and revolutionary resources for computations, communications, and data management. Chemists use databases and data mining to suggest molecular structures, quantum chemistry to predict their stability, and statistical mechanics methods to calculate their properties and interactions with other species. This article aims to give an overview of role of information technology in chemical research. It describes how sophisticated simulation tools and techniques of informational technology helps in various aspects of research in chemistry. Description of one noteworthy application of IT is also given highlighting role of IT. It can be concluded that recent development in computers and software open many doors for new research in chemical sciences and providing opportunity in research and development. The chemical sciences in the twenty-first century will include information, computation, and communications capabilities as both assets and challenges.

Keywords: computational chemistry, Chemical Sciences, green chemistry, simulation

1. Introduction

Information Technology, IT is the application of computers and other electronic equipment to receive, store, retrieve, transmit, and manipulate data. This data becomes information when it is put into intelligible and useful forms for communication. Reliable information technology is key to engineering new scientific and chemical developments. Chemistry and chemical engineering are being transformed by the availability of information technology, modeling capabilities, and computational power (Lewars 2024). Information technology provided chemical science and technology with truly remarkable and revolutionary resources for computations, communications, and data management. Sustained mutual growth and interdependence of the chemical and information communities should take account of several unique aspects of the chemical sciences (Dykstra et al 2011). These include extensive and complex databases that characterize the chemical disciplines; the importance of multiscale simulations that range from molecules to technological processes. Computer software has become multiple applications for calculating the chemical properties of many materials in purely scientific fields, such

as thermal and electrical properties, and calculations related to the electronic distribution of some materials, as well as in practical fields such as drug industry and design, environmental and atmospheric chemistry, nanotechnology and materials science (Goh et al, 2017).

1.1 Information and databases - Development of databases, database relationships, data-mining tools and tutorial structures enabled the kind of research to be done in the chemical sciences that could never have been done before. Data-mining algorithms, information technology has permitted all scientists to use the huge resource of chemical data in a highly interactive, reasonably effective way.

1.2. Computing Capability, Integration, and Access – Due to advances in IT quantum chemical calculations of molecular electronic structure, Monte Carlo calculations of equations of state for gases and liquids, or molecular dynamics simulations of the structures of high-temperature and high-pressure phases is possible in chemical research. Integrated models for plant design and control, Monte Carlo models for mixtures, polymer structure and dynamics, and quantum and classical dynamics models of reaction and diffusion systems provide chemical engineers with an ability to predict the properties of complex systems, which was not possible before.

1.3. Bandwidth and Communication Capabilities - The impact of increased bandwidth is key to much of the future societal and educational development of the chemical sciences—to the processes that will allow chemists and chemical engineers to interact and collaborate with one another, with other scientists, with industrial and medical practitioners, and with users that require chemical information, methods, and models. Similarly, increases in network and memory bus speed have made computation a more powerful tool for modeling in chemical science.

2. How Information Technology helps in Chemical research

Information and technology plays a critical role in Chemical research from aiding in solving simple to highly complicated research questions. An abundance of wonderful computer programs and modern graphics, fast calculating software, and simulation techniques are available, and all of these things have elevated applied computational chemistry to a status as one of the major fields of chemistry and chemical engineering in the 21st century.

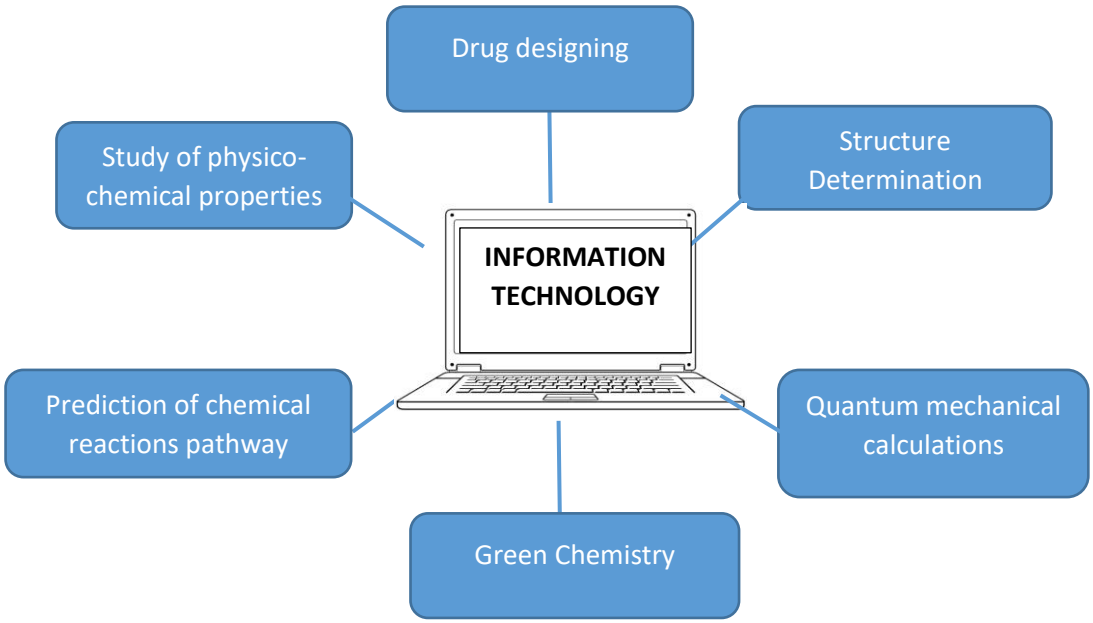

Fig 1. Role of IT in Chemical research

2.1. Computer-Aided Drug Design - This has become a significant contributor in the discovery and development of new pharmaceuticals. Integrated modeling efforts are proving highly valuable to industry in such areas as drug design and properties control. Computer-aided drug design (CADD) offers a more efficient and cost-effective approach, complementing traditional experimental techniques (Mihai et al 2025). Some examples of molecules created with the direct input of computational chemistry include the antibacterial agent norfloxacin, the glaucoma drug dorzolamide and the agrochemical fungicide myclobutanil.

2.2. Simulation and Computational Methods for Design and Operation: These techniques are used for integrated design and real-time optimization of a chemical plant or enzyme inhibitors. Predictive capabilities are now good enough to obtain phase diagrams for real gases with accuracies exceeding most experiments. Simulations are now beginning to address more complex systems, including polymers, biomolecules, and self-assembling systems. Molecular dynamics (MD) simulation of billions of atoms is now possible, permitting both understanding and prediction of such phenomena as phase and fracture behaviour. Chaban et al, 2022 investigated reaction paths that are responsible for CO_2 chemisorption by the ammonium- and phosphonium-based ionic liquids containing an aprotic heterocyclic anion 2-cyanopyrrolide revealed by the simulations of competing pathway which helped in understanding of the outstanding CO_2 sorption performance of the quaternary ammonium- and phosphonium-based 2-cyanopyrrolides.

2.3. Chemoinformatics: Chemoinformatics is a new branch of Chemistry which is defined the "application of computational techniques to the discovery, management, interpretation and manipulation of chemical information and data. It is a strong growth area in IT for its ability to use fundamental knowledge to yield practical advances in the field of Chemistry. Regarding structure representation and database construction, the digital representations of polymers are the predominant methods in cheminformatics along with some newly developed methods that integrate the polymeric multiscale structure characteristics. Zhang et al , 2016 carried out computational and experimental studies to reveal the origin of the meta-selectivity of Cu-catalyzed arylation of anilides and α-aryl carbonyl compounds using diaryliodonium salt as the aryl source because Pd catalyzed arylation of anilides under similar conditions gives the ortho product.

2.4. Molecular Electronic Structure Calculations: This technique of information technology can model the structure and properties of a given molecule to high accuracy for chemists. This ability has led to a new way of doing science, based not on artificial models but on accurate quantum calculations of actual chemical species. It is helpful especially in transition state structure which is not accessible for a direct experimental study. Computational chemistry is well suited to the mechanistic studies of chemical reactions (Cheng et al 2015).

2.5. Designing New product - IT has critically important role in designing new products. The dielectric, mechanical, and thermal properties of a large group of polymers were predicted computationally in order to identify a much narrower group of targets on which synthetic efforts were focused. In some cases, accurate calculations can replace experiments that are expensive or dangerous or chemicals. The biosynthetic pathways of natural products are complicated, and it is difficult to fully elucidate their details using experimental chemistry alone. In recent years, efforts have been made to elucidate the biosynthetic reaction mechanisms by combining computational and experimental methods. Biosynthetic studies using computational chemistry for various terpene compounds such as cyclooctatin, sesterfisherol, quiannulatene, trichobrasilenol, asperterpenol, preasperterpenoid, spiroviolene, and mangico has been done (Sato, H. (2024).

Table1. Some of the applications of IT in Chemical sciences research

S.N.	RESEARCH WORK	APPLICATIONS	RESEARCHERS
1	Identification of potential drugs for COVID 19 using molecular docking	Remdesivir was identified and proposed as a potentially effective treatment for its ability to target the RNA-dependent RNA polymerase (RdRp)	Abdo A. Elfiky (2020)

2	Organic Solar cell research	Information obtained about intrinsic properties using IT can be utilised to screen high-efficiency molecules to accelerate the development of organic solar cells.	Cui, Y., Zhu, P., Liao, X., & Chen,Y (2020)
3	Three dimensional protein structure using simulations	Predicts protein structures with atomic accuracy even in cases in which no similar structure is known. Used for determining protein structures to near experimental accuracy in a majority of cases.	Jumper, J., Evans, R., Pritzel, A. et al (2021)
4	Sensitivity of graphene based sensors using computational Chemistry	Provide insights into the fundamental chemical and physical processes behind the measured signal, exploring the scope of possible analytes and prescreening designed sensing materials.	Piras, A., Ehlert, C., & Gryn'ova, G. (2021)
5	Investigation of Hg(II) analysis in real samples using a computational Chemistry approach	Development of procedure to separate and preconcentrate Hg(II) ions in water and vegetable samples by green supramolecular solvent.	Nail Altunay et al (2021)
6	Trapping of Ag^+ into a Perfect Six-Coordinated by Quantum Chemical Calculations and Electrochemistry	Formation of new complex, $(Bu_4N)_2[\beta\text{-}\{Ag(dpp\text{-}bian)\}_2Mo_8O_{26}]$, indicating a unique Ag coordination environment with rich electrochemistry which involved both organic components and octamolybdate ligands,which can also be used as catalyst for electrochemical CO_2 reduction.	Komlyagina et al (2022)

3.

Implementation of IT in Green Chemistry research

Information technology has enabled Chemistry to accomplish many significant research work, whether it is a solution to a major fundamental issue or creation of a novel useful material (Mammino, L. (2022). It can be depicted by this wonderful example of polymer production from CO_2 emissions (Tian et al 2022). Green Chemistry research in CO_2 utilization has focused on the reaction of carbon dioxide with epoxides to produce commercially useful polymers or cyclic organic carbonates; which have uses as green solvents (Darensbourg et al 2013). Recent experimental work has been done on the mechanism of the reaction when catalyzed by complexes of Cr^{3+}, Co^{3+}, or Al^{3+}, with bis (salicylaldimine) ligands; the reaction begins with complexation of the epoxide to the metal, followed by ring opening with an anion initiator such as Cl^- or N^{3-}; this is followed by insertion of CO_2 and then alternating epoxide and CO_2 insertion as shown.

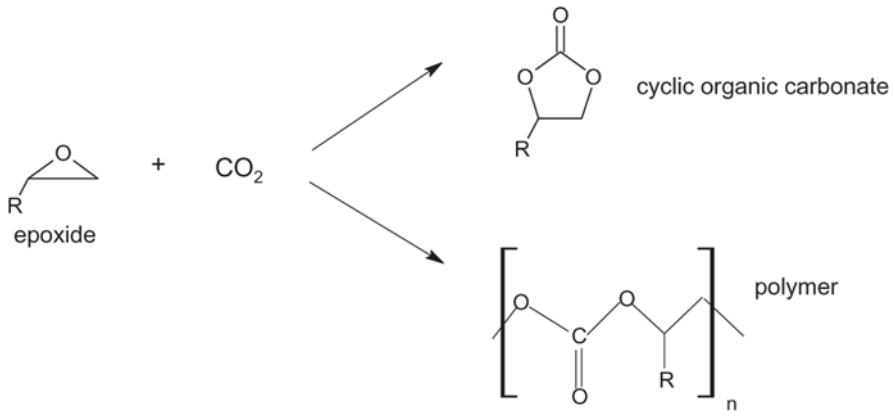

Fig 2. Reaction of epoxide with CO_2

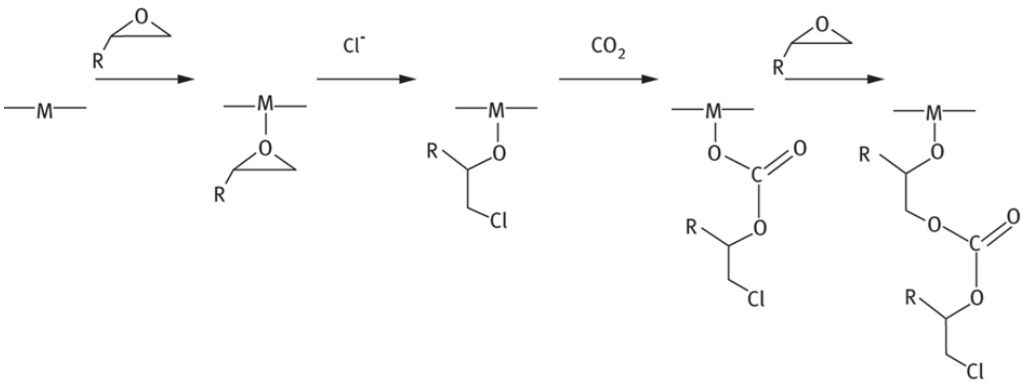

Fig 3. Catalyzed copolymerization of CO_2 and epoxide with initiator Cl^- .

Research in computational chemistry has provided a significant amount of information about this process. Experimental data on the thermodynamics of epoxide formation are little, but a quantum computational study has been made of the thermodynamics of CO_2-epoxide copolymerization, and of the competing process, carbonate formation, for a number of candidate epoxides. Consideration of computational work with experimental data on metal-catalyzed reactions suggests that the competing carbonate formation most likely proceeds from a carbonate back biting reaction which proceeds most rapidly in a "metal-free" fashion as opposed to via a metal complex, (Darensbourg, (2004) as shown.

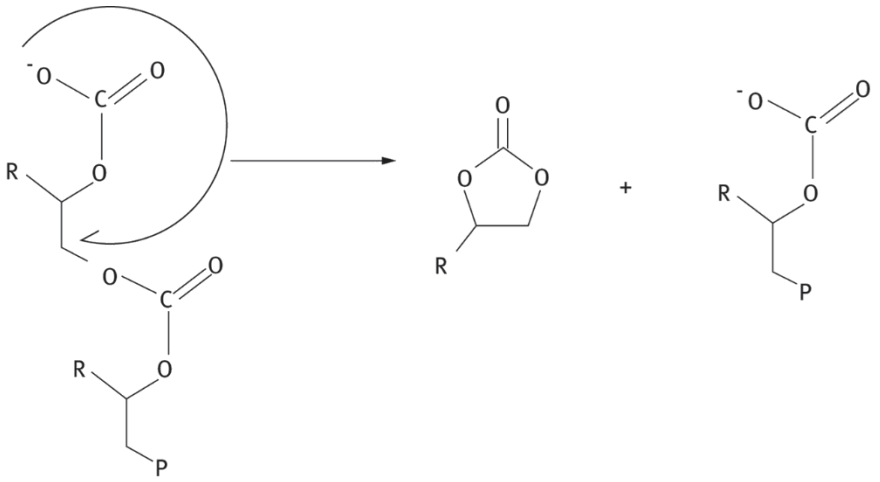

Fig 4. Carbonate "back biting" reaction, "P" represents polymer chain

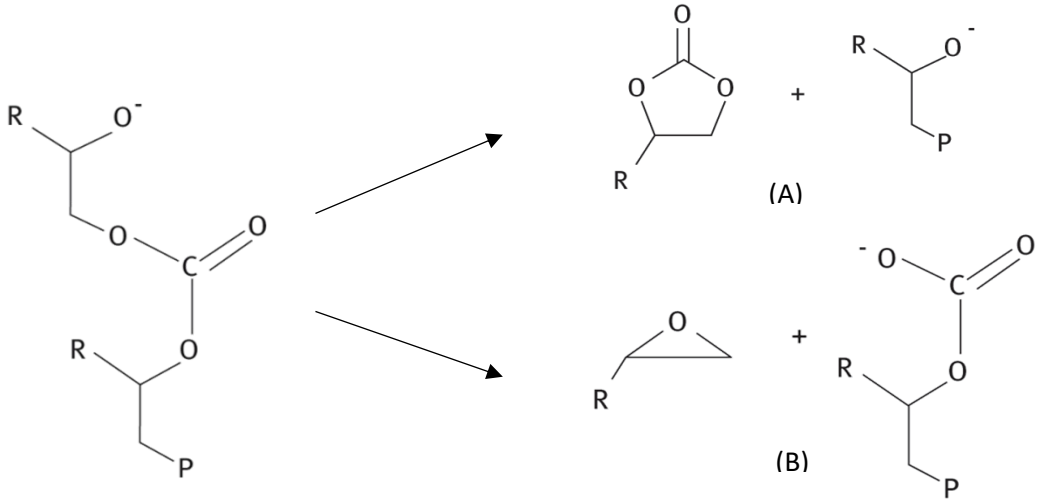

Fig 5. Alkoxide "back-biting" reaction producing (A) a cyclic organic carbonate or (B) epoxide "P" represents polymer chain

Quantum computations determine that epoxide forming reactions are thermodynamically favorable; however, cyclic carbonate is in general the only product because epoxide formation has a higher barrier for reaction. In addition, the epoxide-forming reaction gives rise to carbonate polymers that undergo carbonate back-biting. Study of reaction mechanism was only possible due to IT tools, which was further examined by the experimental results.

Computational simulation using machine learning models can be used in prediction of CO_2 absorption in environmental applications. Computational modeling can be employed for capture of carbon dioxide from gaseous flows to optimize the process and enhance the separation efficiency. Removal of CO_2 as pollutant from gas streams such as air, natural gas (NG), etc. is of great importance. The used machine learning models indicated to be robust for simulation of CO_2 absorption in liquid phase for environmental applications and can be used to save time and costs of measurements (Darensbourg, 2015). Utilizing sustainable monomers and the development of polymers that can be chemically recycled/degraded is an essential target of chemistry in the 21st century. Polycarbonates synthesized from the ring-opening copolymerization (ROCOP) of epoxides and CO2, and polyesters synthesized from the ROCOP of epoxides and anhydrides are sustainable plastic materials. Designing efficient catalysts for these processes remains challenging. Kinetic and structure−activity studies that underpin the performance of these catalysts are done by computational methods (Diment, 2022). Computational chemistry has been an important contributor to green chemistry.

4. Challenges in use of information technology

The integration of information technology (IT) in chemistry is a rapidly evolving field that presents several challenges. One of the primary hurdles is the development of standardized data formats and ontologies that enable seamless data exchange and integration across different systems and laboratories. The lack of standardization leads to data silos, making it difficult to share, compare, and analyze data, ultimately hindering the advancement of scientific research. The vast amounts of data generated by high-throughput experiments and simulations require advanced data analytics and machine learning techniques to extract meaningful insights (National Research Council, 2003). However, the complexity of chemical data and the need for domain-specific knowledge make it challenging to develop effective data analysis tools.

Another significant challenge is ensuring the accuracy, reproducibility, and reliability of computational models and simulations. Small errors or inaccuracies in these models can have significant consequences, such as incorrect predictions or misinterpretation of results. Therefore, it is essential to develop robust validation and verification protocols to ensure the quality of computational models. Additionally, the increasing use of cloud computing and big data analytics in chemistry raises concerns about data security, intellectual property, and collaboration. To overcome these challenges, researchers and developers must work together to establish standardized data formats, develop advanced data analysis tools, and create robust validation protocols. Moreover, there is a need for education and training programs that equip chemists with the necessary IT skills to effectively utilize computational tools and methods. By addressing these challenges, the integration of IT in chemistry can lead to significant breakthroughs in fields such as drug discovery, materials science, and environmental chemistry.

5. Conclusion

Information technology holds great potential to advance the rapidly growing field of computational Chemistry. It helps to understand chemistry and to predict promising directions that experimentalists can follow to make new discoveries. The impacts of computations can be seen on the understanding of mechanisms and selectivities, especially in the organometallic, biosynthetic, and materials fields. Experimentalists often turn to computational chemists for help with understanding how their chemistry works or to predict how to overcome problems encountered experimentally. Green approach of finding uses for CO_2 as a feedstock for syntheses of chemical products depicted in this paper is a good example.

IT also aids to undertake the development of conceptual models to understand factors controlling reactivity such as the Activation Strain or Distortion/Interaction Model, the nature of transition states such as aromaticity, or the general relationship of electron densities to reactivity, as in Conceptual Density Functional Theory. In future it is expected that IT will rise as a very helpful tool covering a wide range of Chemical research to give fast and accurate results.

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