iJRASET
International Journal For Research in Applied Science and Engineering Technology

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 7 **Issue:** X **Month of publication:** October 2019

DOI: http://doi.org/10.22214/ijraset.2019.10011

www.ijraset.com

Call: 08813907089 | E-mail ID: ijraset@gmail.com

International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.177
Volume 7 Issue X, Oct 2019- Available at www.ijraset.com

Review of Artificial Intelligence Driven Chemistry

Aryan Yashvardhan Sharma[1], Rohan Sahni[2], Sarvjeet Herald[3]
[1, 2, 3]*RoboGenius, India*

Abstract: ***From discovering new drugs to autonomous laboratories in Chemistry, impact of AI will be huge in the coming years. To understand the philosophy and trend of how AI is transforming the discipline and introducing new dimensions, we start from reviewing the history of Artificial Intelligent systems in Chemistry, how it has evolved over the time and penetrated into different subdisciplines of Chemistry and is being adopted across multiple sectors of industry. We also discuss changing the job roles of the professionals and identify that new jobs will be created especially related to data management and production.***
Keywords: Artificial Intelligence, Chemistry, Retrosynthesis, Molecular Modelling, Structural Elucidation, Machine Learning, Neural Networks, Deep Learning

I. INTRODUCTION

When we hear about Chemistry, we think of colourful chemicals mixing with each other or making new drugs by combining different compounds, looking for patterns and regularities in what we already know. But media coverage and public discussions about Artificial Intelligence (AI) is almost impossible to avoid today, even in Chemistry. Be it Synthesis Design Systems for the simulation of chemical reactions, the Structure Elucidation Systems for the interpretation of spectral data, the Molecular Modelling Systems for the visualization of chemical structures and the calculation of physicochemical parameters.

It is understandable that people interested in Chemistry are excited about understanding the intersection between AI and Chemistry. Since Chemistry is a very old discipline, this article is aimed at people who are interested in understanding unprecedented transition in Chemistry with the introduction of AI, a term which was coined in the year 1956 with the aim to enable computers do things which people do better. This includes ability to think and act like humans, ability to learn, identify and solve problems like humans and reason and move like humans. Eventually ends up doing all things that human do and in a much better way. Thus, providing an entirely new perspective of the future in the age of cyber-physical convergence. In this article will review how these different areas of research in chemistry got boosted with the help of computers so far, how AI got involved in their research and where this AI-driven chemical research is heading in order to get an insight to adoption of AI in industry and the changing roles of the professionals. Section II provides brief overview of the history of AI Systems in Chemistry, Section III provide insight into the current research landscape in the Chemistry discipline with AI, Section IV looks at adoption of AI in subdisciplines of Chemistry, Section V shares the revolution across industry sectors, Section VI provides light on the changing roles of the professionals in the discipline and finally Section VII concludes this article with the challenges which will are likely to become reality in the future.

II. HISTORY OF ARTIFICIAL INTELLIGENT SYSTEMS IN CHEMISTRY

Early intelligent systems focused on solving Chemical Engineering design problems and processes. They employed symbolic manipulation, data structures or intelligent systems for mimicking the problem-solving ability of a human being with expertise in the given domain but relied on predetermined set of rules. By expertise, we mean, large amount of domain knowledge and heuristics built over the years of experience in the professional practise. Computational flexibility in terms of overcoming the reliance on predetermined rules in the early systems was attempting by separating the knowledge base from the search base, but still it required extensive time, effort and money to develop a credible intelligent system to tolerate complex nature of the scalable industrial applications.

CONPHYDE for example, was used by chemical engineers in selecting the appropriate vapour -liquid equilibrium for performing process simulations. It asked questions in an intelligent sequence consisting of predetermined rules and provided advice to the engineers. Adaptive Initial Design Synthesizer System which employed intelligent methods such as symbolic manipulation, means-to-ends analysis and data structures was used for systematic process synthesis methodology. Auto Deductive Systems are intended to assist chemist in the design of experimental strategies which had been traditionally regarded as the important goal in Computer Chemistry. Chemical Reaction Analysis and Modelling System (CRAMS), for example, is one of the first and most powerful numeric Auto Deductive Systems designed to aid Chemists in optimizing the number of measurements in rate or equilibrium controlled chemical reactions. Its input is user-friendly and chemical equations are coded and are augmented with indications to steer the code execution into a predictive or a computational model. Similar systems employed stimulus-response model of cognition, and pattern-matching and search model of symbolic computation [12].

Limitation on the data and lack on powerful computing resources were important hindrances to advance the early technology for developing artificially intelligent systems which can learn, identify and solve problem similar to a well-trained experience chemical engineer. But towards end of 20th century, as computing resources started to appear in abundance, the introduction of Machine Learning, Neural Networks and Deep Learning reignited the interest to advance technology and started to create new opportunities.

Machine learning techniques and neural networks allowed backpropagation to self-learn hidden patterns in the data. This led to development of, for example, materials design systems like gasoline additives, formulated rubber and catalyst design; domain-specific representations and languages, modelling environments; molecular structure search engines; automatic reaction network generators; chemical entities extraction systems; predicting electronic structure correlation energies. California Institute of Technology, for example, developed a system to predict chemical reactions long before reagents hit the test tube. University of Cambridge is addressing the same by remodelling chemical reactions as a machine translation problem. Yale, for example, developed a robust computational catalyst design system using inverse design methods which benefits from Machine Learning techniques and scoring functions to provide patterns of molecular correlation to catalytic properties to find catalysts and predict which compounds can create materials before setting foot in the lab [9]. University of Glasgow is developing software to design and 3-D print small, portable reactors to provide manufacturing of specific molecules on-the-go. Such disposable or recyclable reactors could enable much lower cost synthesis of high value and niche-area products, particularly in the austere locations.

Convolutional neural networks, Reinforcement learning, Recurrent neural networks, Statistical Machine Learning, Least Absolute Shrinkage and Selection Operator, Support Vector Machines, Random Forest, Clustering, Bayesian Belief Networks further contributed in advancing the technology. The approach of layer-by-layer training, strategy, convolution in training of the neural nets made feature extraction feasible. Memory Networks were used to formulate reasonable reaction schemes and synthesis strategies. However, data limitation used for training the intelligent systems and its quality, remains a problem. But stimulations are used as an alternative. For example, in material science applications, simulation of a reaction in a forward search is strongly dependent on the quality of the reactivity function, which undergoes steady improvement by the inclusion of new experimental data in the reactivity space.

III.CURRENT RESEARCH DRIVERS OF AI-DRIVEN CHEMISTRY

We have broadly identified three academic research areas which leading technical advances at the intersection of Artificial Intelligence and Chemistry and have implications sub-disciplines of chemistry. These are Retrosynthesis, Molecular Modelling and Structure Elucidation.

A. Retrosynthesis

Retrosynthesis is focused on identifying different possible ways in which chemical reactions are needed and the sequence to retrieve a specific compound as the outcome. In order to successfully synthesize a specific drug or an organic molecule, the best way is to work backwards from the final product and discover the reaction route. This includes gaining access to database of existing possible chemical reactions and identifying algorithm to make new molecules.

B. Molecular Modelling

Molecular Modelling includes perception, manipulation, physicochemical parameterization and visual reproduction of molecular structures by a artificially intelligent computer program. Principal information about molecular structure can be perceived and understood more easily when presented in the chemist's most familiar language. That is, by a picture of its structure using molecular graphics techniques instead of a list of numbers. Many methods have been developed to introduce information about a two-dimensional or three-dimensional molecular structure into a computer program, for example, using input symbols, graphical or alphanumeric, which are further translated into an internal representation by a set of rules that simulate the human perception of a molecular image. The most direct way to obtain 3-D information about a known molecular structure is to access a crystallographic data bank which records the X-ray crystal data of compounds for retrieval.

C. Structure Elucidation

Structure-generating algorithms have characterized the birth of computational chemistry and structure elucidation systems. Structure elucidation is a combinatorial or semantic problem which deals with a finite number of atoms that has a finite number of solutions. Early processes of structure assembly were based on a stepwise expansion of the molecular graph, through which a substructure is gradually enlarged to form a complete final structure. Computer-Aided Structure Elucidation and automated structure elucidation system for organic compounds (CHEMICS) are the results of many years of effort in the design of fully automatic and self-deciding structure elucidation systems.

ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.177
Volume 7 Issue X, Oct 2019- Available at www.ijraset.com

IV. ADOPTION OF AI IN CHEMISTRY SUBDISCIPLINES

We have identified seven major subdisciplines of Chemistry which are leveraging Artificial Intelligence: Organic Chemistry, Inorganic Chemistry, Biochemistry, Physical Chemistry, Theoretical Chemistry and Analytical Chemistry. These are discussed in this section.

A. Organic Chemistry

Synthesis of organic molecules remains one of the most important tasks in organic chemistry and the standard approach involved by Chemists is to solve a problem based on their experience, heuristics and rules of the thumb. When Chemists manually design a new drug, they not only need to design a target molecule but also need consider reaction pathways to synthesize it. They usually work backwards, starting with the molecule they want to create, followed by analyzing by a process known as retrosynthesis as discussed in the previous section, in which readily available reagents and sequences of reactions could be used to produce an outcome.

Researchers have tried to show that organic chemistry has a structure similar to a natural language and that the concepts of linguistic-based analysis could be used to also analyze molecules, their patterns of reactivity and their organic synthesis in the hope that Sequence-to-Sequence models for retrosynthesis and reaction prediction will be feasible in future. In this avenue, for example, IBM's neural network model trained on a dataset of 395,496 reactions has learned about prior reactions and is being used to predict what would occur under new experimental conditions.

B. Inorganic Chemistry

The variable spin, oxidation state, and coordination environments favoured by elements with well-localized electrons provide a great opportunity for tailoring properties in catalytic or functional (e.g., magnetic) materials and add layers of uncertainty to design strategy.

The High Throughput Screening uses quantum chemistry calculations to predict material properties, however, the computational complexity of these calculations often imposes a prohibitively high cost on the search for the desired material. This critical bottleneck is resolved by using deep Gaussian process-based approach to develop an emulator for quantum calculations.

C. Biochemistry

Biochemical research generates massive amounts of data which needs to be analyzed, integrated, and interpreted. The need is to create a computer-enabled system that would allow biochemists without deep knowledge in carbohydrate chemistry to gain quick access to well-defined glycan assemblies and also methodology to produce large, well-defined macromolecules with programmable shape, size, and chemistry that combines reactor engineering principles and controlled polymerizations. Artificial Cells will investigate how to design artificial molecules and artificial reaction to enable the cell to solve problems [8].

D. Physical Chemistry

Problems addressed and approaches used in Physical Chemistry are diverse. Knowledge bases can be used for storage and retrieval of databases of vapour pressures of gases or of intermolecular forces and the laws relating to physical sciences. When coupled with an Artificial Intelligence system will be able to solve quantitative problems directly by linking together code, formulas and data in the correct sequence to obtain solutions.

Neural network representation of an alloy can be developed to predict composition and temperature-dependent surface segregation through Monte Carlo models or use Gaussian Process approach for representing the potential energy surface which are useful for reactive scattering calculations and also can relate observed X-ray absorption near edge spectra to nanoparticle structure and composition. Researchers are using Artificial Intelligence approach to reduce the number of structures needed to be computed to arrive at a Density Functional Theory based free energy diagram in which neural networks are trained to study the performance of fourth-order gradient expansions of the Kinetic Energy Density in semi-local kinetic energy functionals depending on the density-dependent variables

E. Theoretical Chemistry.

Be it Feynman diagrams in Physics or the structural elucidation in chemistry, theoretical problems can be addressed by solving graphs. A deep generative model known as SELF-referencIng Embedded Strings, for example, are applied to represent chemical structures for molecules using semantically constrained graphs, SMILES, in a simple, robust, deterministic, domain-independent, model-independent way. SELFIES are based on a Chomsky type-2 grammar, augmented with two self-referencing functions for generation of valid graphs for a domain- and model-specific applications. [11]

F. Analytical Chemistry

In Analytical Chemistry, attention is given to the approaches based on problem-reduction search methods, algorithmic and heuristic, in the elucidation of the structure of complex organic compounds by sophisticated computer program systems and deep learning techniques to allow better quality data to be extracted. For example, integrating and analysing multi-omics (genomics, transcriptomics, proteomics, metabolomics, metagenomics*)* data, identifying a dozen of neurotransmitters in a single experiment are important research topics in analytical chemistry.

V. AI REVOLUTION IN CHEMISTRY ACROSS INDUSTRY SECTORS

We have identified eight major industry sectors which are currently using Artificial Intelligence: Pharma; Material; Automation; Agriculture, Food and Health; Forensic; Manufacturing; Oil & Energy; and Education and Research. These are discussed in this section.

A. Pharma

There is great heterogeneity in the pathophysiologic factors and processes that contribute to disease, suggesting that there is a need to personalize medicines to the nuanced and often unique features possessed by individual patients. Retrosynthesis have a great role in discovering new drugs by finding different possible ways to get the desired product. The process of drug discovery is usually very complex, time-consuming and expensive as different data have different accuracy, fidelity, format and quality and the cost of maintenance is also high.

Current approaches to deal with these are mainly using Phenotypic Screening with no target knowledge, Target-based design using Nuclear Magnetic Resonance (NMR) or Crystallography to find possible structures of protein molecules or by establishing Quantitative Structure–activity Relationship (QSAR) or Inverse QSAR and High Throughput Screening. Burke Lab, Cronin Lab, Chemspeed, Eli Lilly are taking the lead. However, the goal is to achieve a closed-loop automated discovery platform with no human involvement in the entire process [2].

Artificial intelligence when interlinked with the traditional computational techniques can provide better insight especially for rheological problems. However, the challenge is to integrate different types of data within a single AI framework to limit human bias, increase accuracy and model interdisciplinary nature of medicine. But if achieved, will improve drug discovery, molecular discovery and can provide unprecedented results [5].

B. Material

Issues of data scarcity and the combinatorial nature of materials spaces which limit the application of Artificial Intelligence techniques in materials science can be overcome by using rich databases and emerging AI techniques. In order to solve the data problem, data management systems like Novel Materials Discovery Laboratory which is a user-driven platform for sharing and exploiting computational materials science data is a good path forward. Calculating, for example, all the permutations and phases in the formation of a high entropy alloy or finding out any comprehensive, systemic way of what new and potentially useful behaviours might exist in the combination of elements can open new unknown territories. From this perspective, various projects are being done at Material Measurement Lab at NIST such as JARVIS-ML, Teaching Liquid State Theory to an Artificial Neural Network (ANN) and Material Design Toolkit.

C. Automation

Introducing Automation and Artificial Intelligence in Clinical Labs can lead to the development of new diagnostic and prognostic models and support personalized medicine. Self-learning algorithms can perform diagnosis by integrating all data from an individual. In the context of Materials, progress has been made to produce and characterize smart materials using the most abundant products of the biomass, i.e. polysaccharides which include cellulose, hemicelluloses, chitin, chitosan, and alginates and their by-products. Owing to their low density, thermal stability, chemical resistance, high mechanical strength, biocompatibility, biodegradability, functionality, durability and uniformity, these products are materials of choice for the preparation of smart products that can be used in the very promising areas of nanotechnology, foods, cosmetics and medicine (mainly controlled drug release and regenerative medicine) and hance has potential to open new commercial markets in the context of green chemistry.

D. Agriculture, Food, Health

Combined approach of utilizing Low Field-NMR and Backpropagation-ANN has a great potential in Intelligent Online Monitoring and Control Applications for Carrot drying [15]. For example, NMR signals are passed as input variables, followed by a Back Propagation-ANN model for optimization by a transfer function, training function and the number of neurons to model for

understanding the moisture content as an output of AI system. In Sugarcane mills, production of high-quality sugar using ANNs combined with colour information from Digital Images are be used to predict the content of sugarcane stalks in the presence of a solid impurity.

Use of Bioinformatics predictive methods based on ANN at different steps of the olive oil production process, which includes olive tree and fruit care, fruit harvest, mechanical and chemical processing, and oil packaging have been examined in-depth with a view to their optimization and so have the authenticity, sensory properties and other quality-related properties of olive oil. Artificial intelligence smelling using Sensomics-Based Expert System are used to determine Food Odour Codes [6].

E. Forensic

New devices are emerging for predicting Post-Mortem Interval or time of death by identifying biomarkers in different biological fluids such as blood, urine by analysing profile of different metabolites in the blood such as Lactate dehydrogenase LDH, Aspartate aminotransferase AST, triglycerides and cholesterols. In addition to this is measurement of blood pH. The use of such biochemical markers could be promising tools in forensic death investigations.

F. Manufacturing

A new learning algorithm developed at New York University, for example, can predict behaviour of a molecule known as malonaldehyde that undergoes an internal chemical reaction to build a knowledge base about atomic interactions within a molecule and then draws on that information to predict new phenomena. This can aid in the development of pharmaceuticals and can be used to enhance the performance of emerging battery technologies, solar cells, and digital displays.

G. Oil & Energy

For efficient energy generation, Artificial Neural Networks are used for optimization of Solid Oxide Fuel Cells by controlling anode feeding composition, the equivalent hydrogen flow rate per unit cell active area, current density, temperature etc so that they can be effectively used for stationary power generation in homes, vehicles, factories etc [4]. Drones combined with high-resolution digital imaging and softwares like Petroleum Analytics Learning Machine can together work as a real-time intelligent system which can be deployed as Methane/Ethane gas analyser for monitoring pipeline and report can comprise of logs which shows the accurate flight-path along with GPS coordinates for forecasting and optimizing production from the data collected for better operating performance [1].

H. Education and Research

AI can also enhance online teaching platforms using the concept of Virtual Laboratories for integrated teaching, research and promoting cross-disciplinary research. One example could be Intelligent Virtual Chemistry Laboratory tool for simulating chemical experiments online using naive Bayes algorithm.

The tool presents an easy to use web-based interface, which takes as input the reactants and presents results in the form of type of reaction occurred and the list of possible products

Since Autonomous Laboratories require considerable effort in designing and writing advanced and robust software packages to control, orchestrate and synchronize automated instrumentations, cope with databases and interact with various artificial intelligence algorithms. Harvard has introduced ChemOS, which is a portable, modular and versatile software package, that supplies the structured layers indispensable for operating autonomous laboratories. It also enables remote control of laboratories, provides access to distributed computing resources, and comprises state-of-the-art machine learning methods.

From the Research perspective, a university department is using AI in AstroBiology and Astrochemistry for their research projects to understand formation of prebiotic molecules in interstellar matter origin of life and for formation of interstellar giant molecules in star-forming clouds. Such experiments are important path forwards to detect most important biomolecules and their precursors that could provide clues on the origin of life.

VI. CHANGING ROLES OF PROFESSIONALS IN CHEMISTRY WITH AI

AI can augment the productivity of professionals, but it can also replace the work done by professionals and will require change in the skillset from mere automation of knowledge discovery to enhancing decision-making by humans. In this section, we attempt to project addition of new duties with the introduction of AI for Chemists, Pathologists and Entrepreneurs including managers and decision makers in the pursuit that other professional roles and job descriptions are also likely to affect which are not covered in this section.

ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.177
Volume 7 Issue X, Oct 2019- Available at www.ijraset.com

A. Chemists

Let's say Chemists are using AI developed by MIT that can generalize to new molecules that have never been made. Chemists can convert this into an executable recipe file and loaded it on to a platform where a robotic arm assembles modular reactors, separators, and other processing units into a continuous flow path, connecting pumps and lines that bring in the molecular ingredients. They then review the suggested synthesis routes produced by the software to build a more complete recipe for the target molecule [14].

B. Pathologists

Pathologists can refer to Molecular Modelling Research for predicting the function of a compound by looking at the 2-D chemical structure for every known metabolite. Combining an advanced live-cell imaging algorithm and artificial intelligence, they can profile cancer cell extravasation within a microfluidic blood-brain niche chip to detect the minute differences between cells with brain metastatic potential and those without.

C. Entrepreneurs including Managers and Decision Makers

Artificial Intelligence, for example, has guided to rapid discovery of three new glass-forming systems. It has also provided us with a quantitatively accurate, synthesis method–a sensitive predictor for metallic glasses that improves performance with use and thus promises to greatly accelerate the discovery of many new metallic glasses. Entrepreneurs including Managers and Decision Makers can use AI to rapidly produce new personalized products, take deployment decisions and command high return on their investments in a comparatively less time than doing it manually.

VII. CONCLUSION

Historically labour intensive and repetitive jobs are not employing AI so that professionals can rapidly they drill down the wealth of insightful data and make new discoveries. However, maintenance and processing of high-quality data for training Artificial Intelligence Systems is still a very challenging. A new profession of data curators is likely to emerge in future.

As Hardware limitations has almost diminished with the Cloud Computing, new avenues of research are being opened. For example, a large collection of computational chemistry databases which includes data from sixteen different research groups across the world for a total of 44,931 unique reference data points, all at a level of theory significantly higher than density functional theory and covering most of the periodic table, to newly developed reaction energy databases and a new collection of databases containing transition metals are emerging. However, higher commitments from individuals and institutions to work together in establishing acceptable procedures for data curation, monitoring, usage, privacy and regulation are required.

More initiatives like DARPA's Make-It program, Chematica Program, Synthia Software to introduce AI in the curriculum to introduce programming environments required to address such challenging problems are encouraged to explain the concepts of deep learning to chemists and other professional roles utilizing the knowledge of Chemistry discipline along with diverse applications, their future potential and changing roles. This will foster the growing movement of AI accelerated chemistry.

Classical computing methods fail not only quantitatively but also qualitatively in the description of the electronic structure of the molecules. Thus, advancement in quantum computing will further accelerate the discipline, but not limiting to discovery of better batteries, better solar panels, better fertilizers and better medicines. Optimizations in the processes using AI will certainly improve efficiency and decrease costs.

Discovery of new drugs will be an achievement for investment of time and resources of scientific talent around the globe. Soon we are entering a world in which we can develop a new therapeutic solution in a matter of days for emerging threat or disease, rather than taking several years. And not only develop a therapeutic that is safe and effective to use, but one can also develop a stable and scalable methods of production in a matter of days.

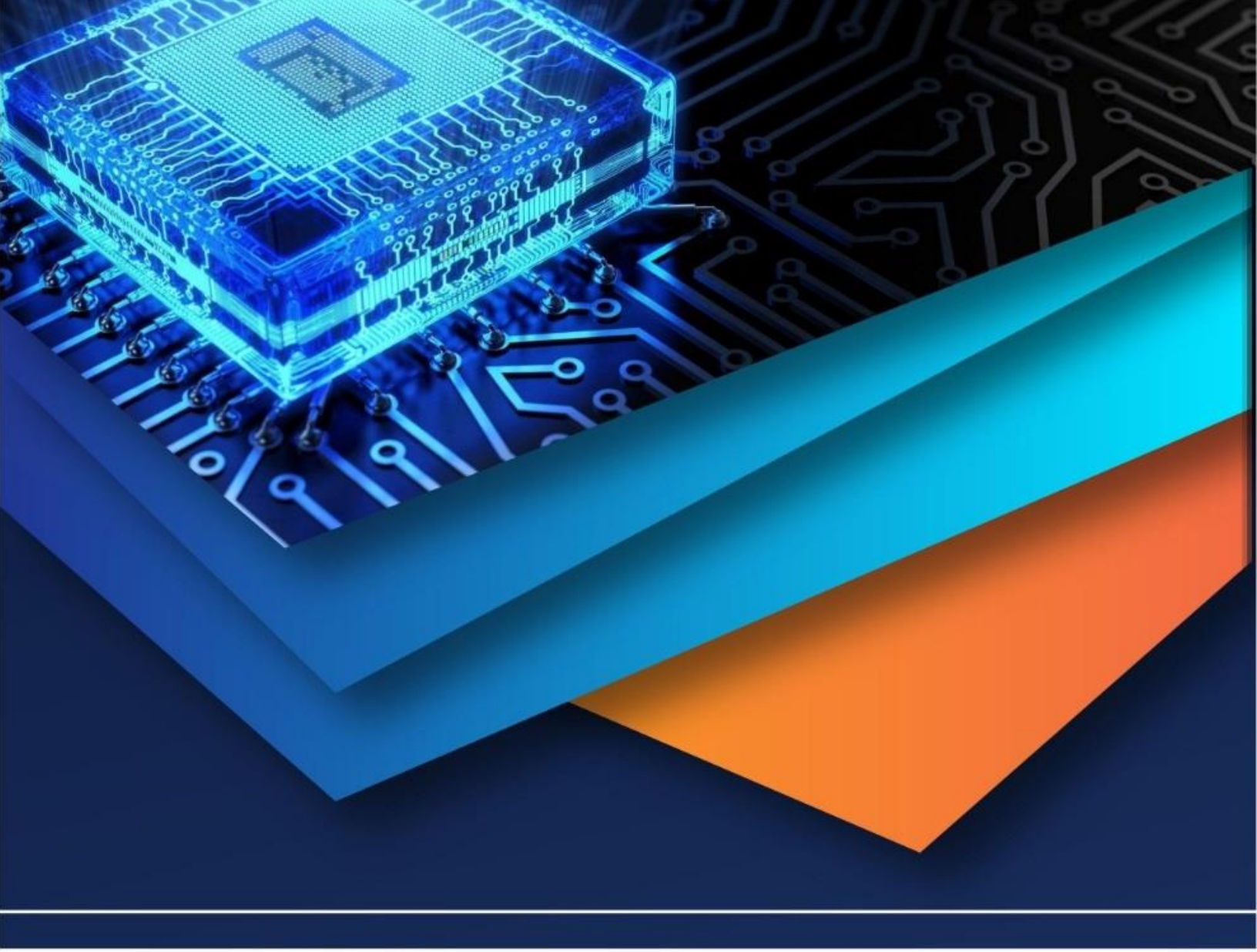
The gap between AI and Chemistry is blurring. It has penetrated in to different subdisciplines of Chemistry and is now being widely adopted in industry. As a result, new discoveries are being made which would have been previously labour some and unknown. Even the roles of professionals are changing.

There is a growing need for them to understand AI and its usage in their professions for productively collaborating with the technology. Focus should be given to the process of data production, curation, cleaning to further enhance the AI and these may emerge as new careers in the discipline.

AI is has taken a leap in the Chemistry. It is guiding the future of the discipline and opening new possibilities.

REFERENCES

[1] R. Anderson, "'Petroleum Analytics Learning Machine' for optimizing the Internet of Things of today's digital oil field-to-refinery petroleum system", in IEEE International Conference on Big Data (Big Data), 2017, pp. 4542-4545.
[2] A. Basile, A. Yahi and N. Tatonetti, "Artificial Intelligence for Drug Toxicity and Safety", Trends in Pharmacological Sciences, vol. 40, no. 9, pp. 624 - 635, 2019.
[3] A. Sohail, M. Fatima, R. Ellahi and K. Akram, "A videographic assessment of ferrofluid during magnetic drug targeting: An application of artificial intelligence in nanomedicine", Journal of Molecular Liquids, vol. 285, pp. 47-57, 2019.
[4] A. Baldinelli, L. Barelli, G. Bidini, F. Bonucci and F. Iskenderoğlu, "Regarding Solid Oxide Fuel Cells Simulation through Artificial Intelligence: A Neural Networks Application", *Applied Sciences*, vol. 9, no. 1, p. 51, 2019.
[5] C. Gilvary, N. Madhukar, J. Elkhader and O. Elemento, "The Missing Pieces of Artificial Intelligence in Medicine", *Trends in Pharmacological Sciences*, vol. 40, no. 8, pp. 555-564, 2019.
[6] W. Guedes, L. dos Santos, É. Filletti and F. Pereira, "Sugarcane Stalk Content Prediction in the Presence of a Solid Impurity Using an Artificial Intelligence Method Focused on Sugar Manufacturing", *Food Analytical Methods*, 2019.
[7] H. Chan, H. Shan, T. Dahoun, H. Vogel and S. Yuan, "Advancing Drug Discovery via Artificial Intelligence", *Trends in Pharmacological Sciences*, vol. 40, no. 8, pp. 592-604, 2019.
[8] C. Goh, H. Ewe and Y. Goh, "An Artificial Cell Simulator based on Artificial Chemistry", *Proceedings of the 2019 8th International Conference on Software and Computer Applications - ICSCA '19*, pp. 338-342, 2019.
[9] J. Freeze, H. Kelly and V. Batista, "Search for Catalysts by Inverse Design: Artificial Intelligence, Mountain Climbers, and Alchemists", *Chemical Reviews*, vol. 119, no. 11, pp. 6595-6612, 2019.
[10] R. Jr, J. and Florea, L. and de Oliveira, M. Diamond, D. Oliveira Jr and O. N, "A survey on Big Data and Machine Learning for Chemistry", *arXiv preprint arXiv:1904.10370*, 2019.
[11] M. H{\"a}se, F. Nigam, A. Friederich and P. Aspuru-Guzik, "SELFIES: a robust representation of semantically constrained graphs with an example application in chemistry", *arXiv preprint arXiv:1905.13741*, 2019. M. Welborn, L. Cheng and T. Miller, "Transferability in Machine Learning for Electronic Structure via the Molecular Orbital Basis", *Journal of Chemical Theory and Computation*, vol. 14, no. 9, pp. 4772-4779, 2018.
[12] M. Welborn, L. Cheng and T. Miller, "Transferability in Machine Learning for Electronic Structure via the Molecular Orbital Basis", Journal of Chemical Theory and Computation, vol. 14, no. 9, pp. 4772-4779, 2018.
[13] Rau M.A., Zahn M., Misback E., Burstyn J. (2019) Adaptive Support for Representation Skills in a Chemistry ITS Is More Effective Than Static Support. In: Isotani S., Millán E., Ogan A., Hastings P., McLaren B., Luckin R. (eds) Artificial Intelligence in Education. AIED 2019. Lecture Notes in Computer Science, vol 11625. Springer, Cham
[14] S. Saikin, C. Kreisbeck, D. Sheberla, J. Becker and A. Aspuru-Guzik, "Closed-loop discovery platform integration is needed for artificial intelligence to make an impact in drug discovery", *Expert Opinion on Drug Discovery*, vol. 14, no. 1, pp. 1-4, 2018.
[15] Q. Sun, M. Zhang, A. Mujumdar and P. Yang, "Combined LF-NMR and Artificial Intelligence for Continuous Real-Time Monitoring of Carrot in Microwave Vacuum Drying", *Food and Bioprocess Technology*, vol. 12, no. 4, pp. 551-562, 2019.
[16] V. Solinge, W. Ten Berg and M. Haitjema, "Data-driven integrated diagnostics: the natural evolution of clinical chemistry?", *Nederlands tijdschrift voor geneeskunde*, vol. 163, 2019.



10.22214/IJRASET

45.98

IMPACT FACTOR: 7.129

IMPACT FACTOR: 7.429

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY