



# Kreative Chemistry Learning

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Sir Chandrasekhara Venkata Raman  
1888-1970

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## About the journal

Krea University is launching a quarterly, fully online journal to enable undergraduate students and teachers. The major scope of the journal is to communicate ideas that make learning and teaching chemistry enjoyable and insightful. Assisted by a student team, the editorial board will ensure high quality articles that focus on pedagogy are published in the journal. Manuscripts that cover various aspects related to the following themes will be considered.

1. New methods of teaching difficult concepts
2. Teaching chemistry for other disciplines and vice-versa
3. Novel experimental methods, simple alternate experiments
4. Interesting problems that bring out non-obvious features
5. Developments in chemistry research and teaching
6. Applications of chemistry
7. New courses in or relevant to chemistry
8. Ideas for revamping chemistry curriculum, teaching, etc.
9. Summary of experiences in teaching revamped curricula

There are no article publication charges and access to the journal is free. Author instructions and manuscript preparation details will be shared on the journal website.

Cover page illustration: Artistic rendering of Sir CV Raman generated by ChatGPT

### Contact info:

Mail: [krea.chemlearning@krea.edu.in](mailto:krea.chemlearning@krea.edu.in)

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## Editorial

It is a pleasure for us to launch the Krea home journal “Kreative Chemistry Learning” on the occasion of Science Day. It is only appropriate that a scientific initiative such as the launch of this house journal occurs on the anniversary of the announcement of the Raman effect by the illustrious scientist of India, Prof. C. V. Raman. It was on Feb 28, 1928, that Raman announced to the world his discovery which earned him the coveted Nobel prize in 1930. The Raman Effect forms the cornerstone of many investigations in Biology, Chemistry, Physics, Materials and Environmental Sciences, to name just a few.

The study of science is often assumed, particularly in the early years of education, to be an exercise in memorizing facts and providing standard responses to standard questions. Nothing can be farther from the truth. The motivation behind the launch of this journal is to inculcate in students the “4 As” in science learning, i.e. the art of Asking questions, the ability to systematically look for Answers, the skill to make Associations and correlations between seemingly unrelated topics and to develop the confidence and Assurance to defend our conclusions. Raman embodied every aspect of the above traits in his work. Of the “4 As”, the ability to ask the right questions is probably the most important. As it is often said that “The true sign of intelligence is not in answering a question but in questioning an answer”. Raman did exactly that by asking a very simple but profound question on why the sea was blue, which set him off on his journey in understanding light scattering. He was quick to dismiss the then accepted theory of Rayleigh that the sea appeared blue because it just reflected the colour of the sky. He strived to answer the question through carefully designed experiments. When it came time to interpret his findings, he was quick to draw inspiration from the theory of Compton scattering which was reported in 1923 and which had to do with scattering of  $\gamma$ -photons by an electron, where the scattered photon had an energy different from the incident photon. Raman argued that if this were true with  $\gamma$ -radiation, there must be an optical analogue of the same phenomenon. This insightful correlation was what gave birth to the Raman Effect, where too the scattered photon had an energy different from the incident photon. Raman titled his discovery as “A new type of secondary radiation”, which was published in Nature. It is therefore only appropriate that Krea’s house journal is also launched on the day where all these aspects of scientific practice were manifested in that remarkable announcement of a scientific phenomenon.

The Journal will strive to inculcate the “4-As” by publishing articles on various topics in Science by experts in the field. While the Journal is titled as a Chemistry Journal, it will not restrict itself to topics only in Chemistry. It will present topics in related areas which again is to educate the students, that science today does not (and never did) work in isolation. To make this journal accessible to all, the articles in the journal can be accessed free of charge.

In an effort to make the study of science interesting, the Journal will also carry a game corner, where crosswords and puzzles will be presented for students to work on. It will also contain a question corner where a few questions on how science influences our everyday life will be asked. The answers to the questions will be posted in the following issue. To

make the experience interactive, readers will also be encouraged to send in questions that they would like to be answered and appropriate experts will be requested to provide answers to such questions. We do hope that this exercise provides for our young students an enjoyable way to study science. In science, great joy is in the journey undertaken to understand nature; more so than in the answer itself. The answer only provides more, and better questions and the journey begins all over again. Science at its very best, never provides final answers to any question, it provides better questions that can be addressed.

The logo for the journal is a cartoon rendition of the structure of cyanocobalamin (Vit B 12). This logo was chosen as it depicts a major landmark in synthetic organic chemistry. The molecule was synthesized by Woodward and Eschenmoser in 1972-1973 and highlighted the role of teamwork in research. Over 100 chemists were involved in the project which spanned almost 12 years. This molecule also highlights the chemistry-biology- physics connect - a biologically important molecule, whose structure was determined by X- Ray analysis by Dorothy Hodgkin and which was finally synthesized by chemists. We thank Mr. Rithish Bharat and the Communication Team for the logo design.

No effort such as this is possible without the support and participation of fellow academicians. We thank the Vice Chancellor Prof Nirmala Rao for the support she provided for the launch of this journal. The contribution of Prof T. P Radhakrishnan, Prof. K. Sivapriya and Prof. B. Agastya, who enthusiastically submitted articles for the launch of this initiative, is gratefully acknowledged. We also thank the members of the Editorial Board who readily consented to serve on the board and provide us with the necessary support and suggestions. We hope that this journal provides a wonderful learning experience for the young minds in this country.

K S Viswanathan  
Editor

# Emergence and Evolution of Molecular Materials

T. P. Radhakrishnan  
School of Chemistry, University of Hyderabad  
Hyderabad - 500 046, India  
\*Email: tpr@uohyd.ac.in

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**The versatility inherent in the synthesis and assembly that allows the realization of specific materials attributes, makes molecular materials an important class. Design and formation of these materials provide insight into fundamental aspects of structure-function correlations, enabling utilization in several technological applications. This brief overview provides a historical perspective of the origin and evolution of the field of molecular materials, highlighting its relevance, related basic concepts and applications.**

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## 1. Introduction

The emergence of new materials during different phases of history has served as a signature of the evolution of human civilization: the stone age (< 5000 BCE), the copper age (~ 5000 – 3000 BCE), the bronze age (~ 3000 – 800 BCE) and the iron age (~ 800 BCE – 40 CE). The contemporary era is often described as the silicon age, thanks to the dominant use of this element in electronics, and a carbon age with fullerenes, nanotubes and graphene is perhaps imminent. Development of new materials is an integral and essential component of the progress of science and technology, prominently impacting our daily lives.

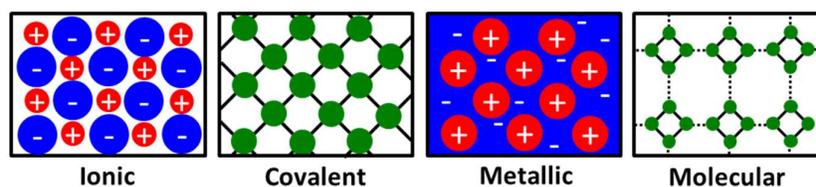
Materials come in many forms with different characteristics and functions, due to their various chemical compositions, as well as the nature of interactions that bind together the atoms, ions or molecules. A broad classification of solid materials based on the latter criterion is shown schematically in Figure 1. Ionic and covalent solids have electrostatic forces or electron pair sharing

bonds respectively, binding the ions or atoms into extended lattices. Metallic solids have a sea of electrons holding the ions together. In molecular solids, strong covalent or coordinate covalent bonds tie together atoms into molecules, and relatively much weaker forces assemble these molecular units into the material. van der Waals, H-bonding,  $\pi$ -stacking etc. are some of the weak interactions that enable the assembly. Common salt (sodium chloride), sand (silica) and iron are examples of ionic, covalent and metallic solids respectively. Ice and urea are examples of molecular solids; the extensive H-bonding interactions that assemble urea molecules into a crystal are shown in Figure 2. Constitutionally, polymers are also molecular materials; covalent bonding of the monomers produces the macromolecules, the assembly of which forms the bulk material.

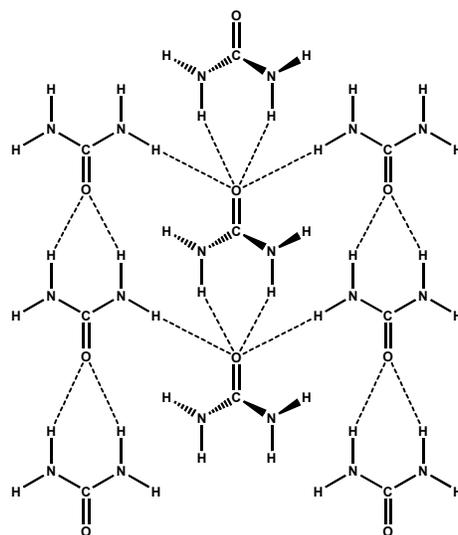
The 2-stage formation of molecular materials provides significant scope for fine-tuning the design and realization of the desired characteristics (Figure 3).<sup>1,2</sup> The first step is

the synthesis of the molecule of interest from atoms or precursor molecules through organic or inorganic chemical routes; the power of synthetic chemistry can be harnessed to prepare molecules with specific properties, as well as functionalities that enable their subsequent assembly. The assembly can be achieved through a wide range of techniques such as simple precipitation and crystal growth, spin-coating of thin films or Langmuir-Blodgett method to form ultrathin films. The relatively weak nature of the assembling forces allows facile deconstruction

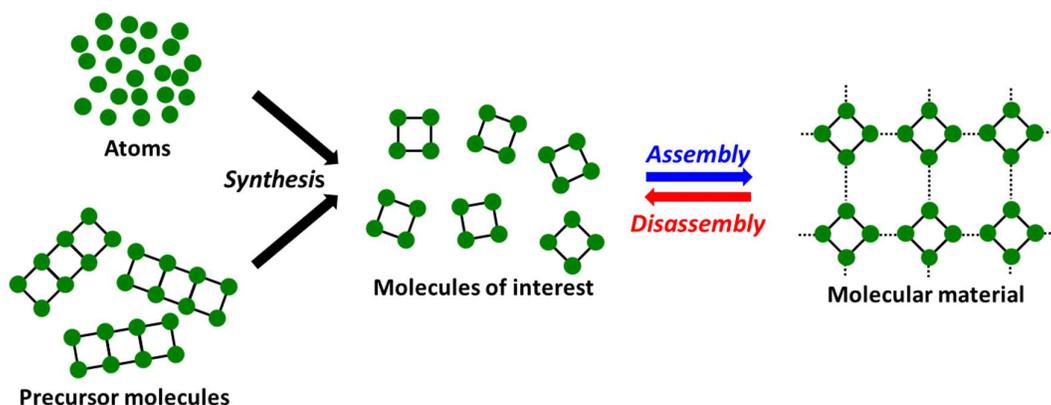
of the material and its reconstruction after modifying the molecular structure or the assembly pathway; an iterative approach can be used to converge upon the targeted materials properties. Subtle changes in intermolecular interactions can have a profound impact on the attributes of the resulting materials, making molecular materials a versatile class in the broad domain of materials science and technology.



**Figure 1.** Schematic 2-D representation of different types of solids: ionic (red circle - cation, blue circle - anion), covalent (green circle - atom, full line - covalent bond), metallic (red circle - atomic nuclei, blue background - sea of electrons), and molecular (green circle - atom, full line - covalent bond, broken line - weak interaction).



**Figure 2.** H-bonding between urea molecules leading to the formation of the urea crystal; note that the middle column of molecules are in a plane orthogonal to that of the two adjacent columns.



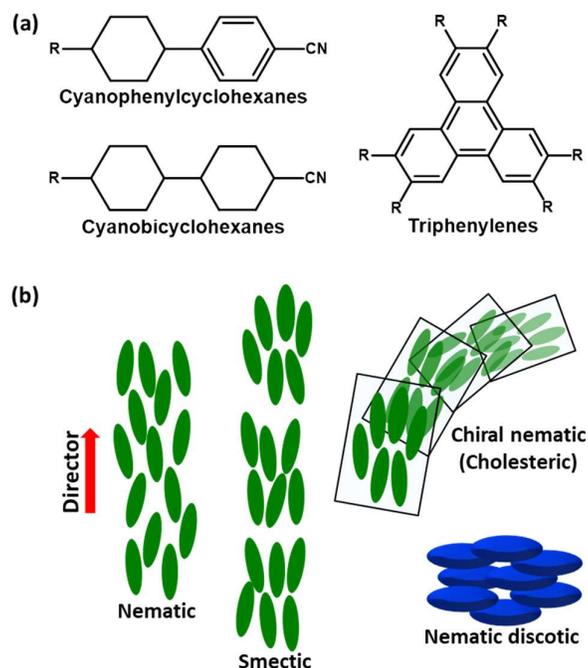
**Figure 3.** Schematic diagram illustrating the 2-stage formation of molecular materials; the full and broken black lines indicate covalent bonds and weak interactions respectively.

## 2. Emergence of functional molecular materials

Functional molecular materials display specific properties that can be exploited to derive useful functions or deploy in devices and technologies. The earliest example of a well-defined class of functional molecular materials is liquid crystals. Reinitzer reported that cholesteryl benzoate is in a peculiar anisotropic fluid state in the range 145.5 - 178.5 °C.<sup>3</sup> Observing a crystalline form coexisting with fluidity, Lehmann described this as a 'liquid crystal' in 1904; exploration of liquid crystals and their applications that followed, has a chequered history.<sup>4</sup> Examples of anisotropic molecules that form liquid crystalline phases are shown in Figure 4a. Some prominent forms of liquid crystals formed by the partial orientational ordering of such molecules are shown schematically in Figure 4b. Thermotropic liquid crystals exist in specific temperature ranges, and lyotropic ones in selected solvent environments. The molecular assemblies lead to high anisotropy in characteristics such as

dielectric permittivity, refractive index and polarizability; sensitive changes in these properties by external stimuli such as electric field, magnetic field or mechanical shear, are exploited in developing important applications like displays (liquid crystal displays, LCDs), sensors and smart windows.

Most of the electrical conductors are based on metals, alloys or metal compounds; organic materials are mostly electrical insulators. A renaissance of molecular materials happened with the discovery of semiconducting behaviour in the charge transfer complex formed between an aromatic hydrocarbon and bromine, by Inokuchi and coworkers in 1954.<sup>5</sup> The non-stoichiometric charge transfer complex, (perylene)Br<sub>x</sub> was found to have a room temperature resistivity of the order of 1 – 100 Ω cm, unusual for any organic material known before. This discovery triggered significant research activity in the field, leading to the development of a wide range of novel molecular materials.

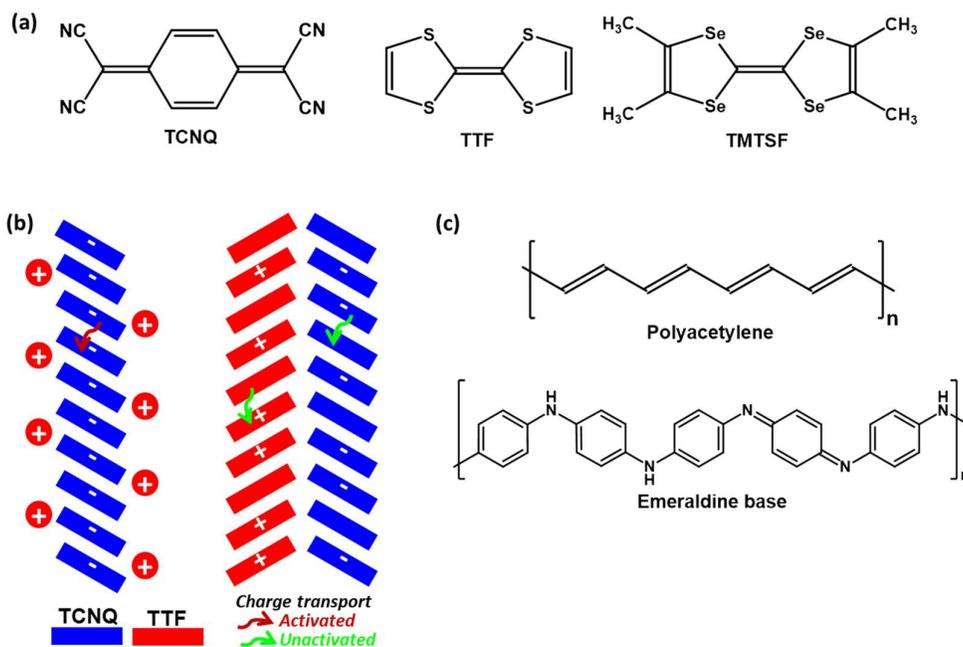


**Figure 4.** (a) Examples of ellipsoidal and disc-like molecules that form liquid crystals (*R* is typically an alkyl or alkoxyalkyl group). (b) Schematic diagram of some common liquid crystal phases formed by: ellipsoid (green) shaped molecules [nematic (partial orientational ordering along the director axis), smectic (additional layered structure), chiral nematic (the director axis of successive layers following a helical orientation)], and disc (blue) shaped molecules [nematic discotic].

### 3. Evolution of functional molecular materials

Several organic semiconductors based on the charge transfer complexes and salts of the  $\pi$ -electron acceptor molecule, 7,7,8,8-tetracyanoquinodimethane (TCNQ) were reported, followed by the discovery of the ‘synthetic metal’, tetrathiafulvalene-7,7,8,8-tetracyanoquinodimethane (TTF-TCNQ, Figure 5a) in 1973.<sup>6</sup> Stacks of the organic molecular ion radicals enable electrical conduction in these materials. If all the molecules in the stack are in the fully ionic form (eg.  $R^+TCNQ^-$ , *R* is usually an alkali metal), the hopping of charges is activated,

leading to semiconducting behaviour; if the molecules have partial ionicity with less than one charge per molecule on an average (eg.  $TTF^{\delta+}-TCNQ^{\delta-}$ ), the charge transport is inactivated and hence metallic (Figure 5b). Many of these organic conductors undergo a phase transition at low temperatures leading to an insulating state; careful design of the molecules incorporating heteroatoms like Se or S enabled the suppression of this phase transition, and manifestation of superconductivity at very low temperatures.



**Figure 5.** (a) Molecular structure of 7,7,8,8-tetracyanoquinodimethane (TCNQ), tetrathiafulvalene (TTF) and tetramethyltetraselenafulvalene (TMTSF). (b) Schematic showing a stack of TCNQ anion radicals with activated charge transport, and stacks in the TTF-TCNQ complex with a partial ionicity of 0.6, showing unactivated charge transport. (c) Structure of polyacetylene, and the emeraldine base form of polyaniline.

The first organic superconductor to be reported was tetramethyltetraselenafulvalene-hexafluorophosphate (TMTSF)<sub>2</sub>PF<sub>6</sub> (Figure 5a); it became superconducting below 0.9 K, under a pressure of 12 kbar.<sup>7</sup> Another major milestone in this area is the discovery of conducting polymers. Polyacetylene (Figure 5c) exposed to iodine vapour was shown to have an electrical conductivity of 38 Ω<sup>-1</sup> cm<sup>-1</sup>, approximately seven orders of magnitude higher than that of the undoped polymer.<sup>8</sup> The principal authors of this work, Shirakawa, MacDiarmid and Heeger were awarded the Nobel Prize in Chemistry in 2000, for this remarkable discovery.<sup>9</sup> Several polymers with extended π-electron conjugation, such as the emeraldine salt form

of polyaniline (protonated form of emeraldine base shown in Figure 5c), doped polypyrrole and doped polythiophene, were shown to be electrically conducting; the protonation or doping introduces charge carriers on the polymer chains and enhances the electrical conduction. Conducting polymers possessing polymer characteristics together with electrical conductivity, find extensive application in sensors, corrosion resistant coatings, display technology etc.

Along with the research on electrical conductors, exploration of molecular magnetic materials also progressed in the latter half of the last century. Ferro and ferrimagnetic materials such as Fe, Co, Ni and

$\text{Fe}_3\text{O}_4$  show spontaneous magnetization (magnetic moment in the absence of an external magnetic field) below characteristic temperatures known as the Curie temperature. For example, Fe becomes ferromagnetic below 770 °C. It was a major challenge to synthesize molecular materials which show ferromagnetism. Extensive research led to the report of the first molecular ferromagnet, decamethylferrocene-tetracyanoethylene (Figure 6a) in 1986.<sup>10</sup> The first purely organic ferromagnet, the  $\gamma$ -phase of *p*-nitrophenyl nitronyl nitroxide (Figure 6a) with a Curie temperature of 0.65 K was reported in 1991.<sup>11</sup> Several small and macromolecular magnetic materials have been developed ever since. Ferroelectric materials show spontaneous electric polarization in the absence of an external electric field, below a characteristic temperature; a popular example is  $\text{BaTiO}_3$ . They are commonly used in sensors, memory devices and capacitors. Some polymorphs of poly(vinylidene fluoride) possessing a polar conformation (one case is shown in Figure 6b) are famous examples of polymer-based ferroelectrics;<sup>12</sup> they also display useful piezoelectric responses, *ie.* production of a voltage upon mechanical stress. A small-molecule based near room temperature ferroelectric, the phenazine – chloranilic acid cocrystal (Figure 6b), is another important discovery in this domain.<sup>13</sup>

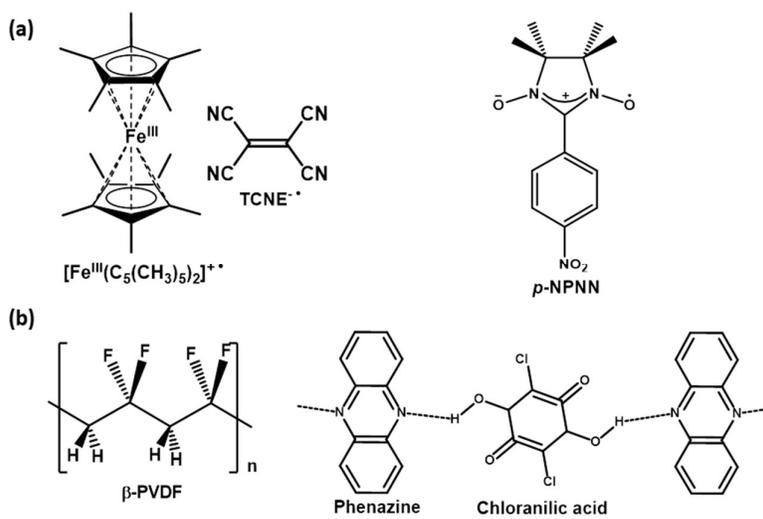
Significant progress has occurred in the domain of molecular optical materials as well. Several families of molecules that show enhanced fluorescence emission in the aggregated and solid state, without the common problem of concentration quenching, have been developed;<sup>14</sup> they find application in areas such as bio-imaging.<sup>15</sup> Electroluminescent materials which emit light upon application of an electric field are critical

for the fabrication of displays (light emitting diodes, LEDs) and sensors; semiconductors such as ZnSe, GaAs, InGaN etc. are commonly used. The mechanical characteristics of molecular materials are a major motivation to develop organic LEDs (OLEDs). Two major landmarks in this direction of research are the demonstration of efficient electroluminescence in *tris*(8-hydroxyquinolino) aluminum<sup>16</sup> and poly(*p*-phenylenevinylene) (Figure 7a).<sup>17</sup> Integral to the development of the burgeoning field of photonics, is nonlinear optical (NLO) materials. The non-linearity refers to the relation of the electric polarization induced in the molecule or material, to the electric field of the incident light, causing a modification in the properties of the material and/or the light during the light-matter interaction. This gives rise to responses such as electro-optic effect and second harmonic generation (SHG); materials such as  $\text{LiNbO}_3$  and  $\text{KH}_2\text{PO}_4$  are well known for such NLO applications. The field of molecular NLO materials began with the observation of SHG in amino acid crystals in 1965.<sup>18</sup> The typical molecular crystal urea (Figure 2) has molecular hyperpolarizability and non-centrosymmetric crystal structure required to exhibit SHG. Active explorations in this domain led to the discovery of materials like N-(4-nitrophenyl)-*L*-prolinol (Figure 7b) which shows highly efficient SHG.<sup>19</sup>

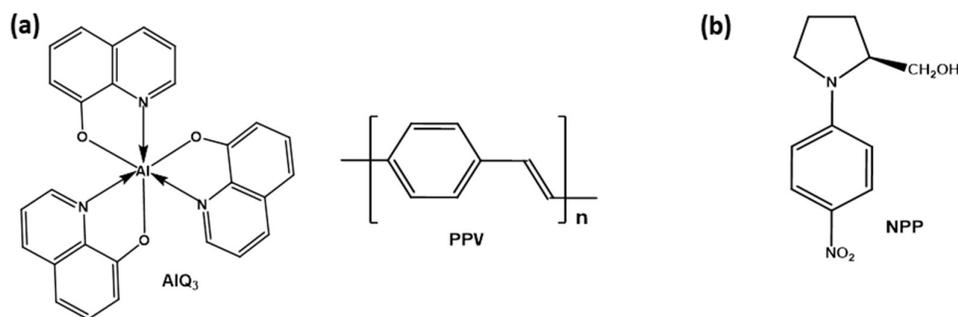
Some of the other important developments that have arisen in the field of molecular materials include the fabrication of molecular nanoparticles with various electronic and optical applications,<sup>20</sup> functional molecular phase change materials<sup>21</sup> etc.

#### 4. Conclusion

This article provides a brief outline of the relevance, emergence and evolution of molecular materials. The domain of



**Figure 6.** Structure of (a) dcamethylferrocene-tetracyanoethylene complex ( $\text{Fe}(\text{C}_5(\text{CH}_3)_5)_2\text{-TCNE}$ ) and  $\gamma$ -nitrophenyl nitronyl nitroxide (NPNN) forming molecular magnetic materials, and (b) poly(vinylidene fluoride) ( $\beta$ -PVDF) and phenazine – chloranilic acid forming ferroelectric molecular materials.



**Figure 7.** Structure of (a) the molecular luminescent materials, tris(8-hydroxyquinolinato)aluminum ( $\text{AlQ}_3$ ) and poly(*p*-phenylenevinylene) (PPV), and (b) the SHG active compound, *N*-(4-nitrophenyl)-*L*-prolinol (NPP).

molecular materials existing at the confluence of chemistry, physics, biology and engineering has led to the unravelling of fundamentally important materials design concepts as well as real world applications. It has spawned new physical models such as those related to charge

carrier transport in low-dimensional systems, magnetic phenomena arising from spin density distributions in molecules, and logical connections between molecular hyperpolarizabilities and material nonlinear optical susceptibilities. Contemporary and futuristic technologies benefit immensely

from different classes of molecular materials including liquid crystals and conducting polymers. The facile tailorability of molecular materials at the molecular and their assembly levels form the basis for expanding their utility and applications.

## ACKNOWLEDGEMENT

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## ABOUT THE AUTHOR



Prof. T. P. Radhakrishnan is an Emeritus Professor (and DAE – Raja Ramanna Chair) at the School of Chemistry, University of Hyderabad. He has mentored research students at various levels, in the broad domains of physical and materials chemistry, and made significant contributions to the areas of molecular functional materials and nanocomposite thin films. He has been involved in teaching at the undergraduate, post graduate and doctoral levels, and has authored the textbook *Core Concepts for a Course on Materials Chemistry* (Royal Society of Chemistry, London, 2022). He is a Fellow of all the major Science Academies of India, Institute for Advanced Studies (Hebrew University of Jerusalem), and the Asia-Pacific Academy of Sciences. He is a recipient of the Swarnajayanti Fellowship, Ramanna Fellowship and J. C. Bose National Fellowship; he was also awarded the Bronze and Silver Medals of the Chemical Research Society of India. He has served as an Associate Editor of the journals, *Resonance* and *Journal of Chemical Sciences* (Indian Academy of Science), and as an Advisory Board Member of *Materials Chemistry Frontiers* (Royal Society of Chemistry).

Website: <http://chemistry.uohyd.ac.in/~tpr/>

# Chemistry: The Central Science

Sivapriya Kirubakaran  
Kankuben Bakshirambhai Gelot Chair, Department of Chemistry,  
Indian Institute of Technology Gandhinagar, Palaj, Gujarat-382355  
\*Email: priyak@iitgn.ac.in

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**"Chemistry begins in the stars. The stars are the source of the chemical elements, which are the building blocks of matter and the core of our subject."**

— Peter Atkins

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## Chemistry The Central Science

*Bridging biology, medicine, environment, and engineering – where **every discovery begins at the molecular level.***



### 1. Introduction

Chemistry is often called the “central science” because it provides a critical foundation that connects other scientific disciplines. From biology and medicine to environmental science and engineering, an understanding of chemical principles is essential for explaining processes and solving problems. However, students outside of chemistry majors often face challenges in grasping these concepts, and educators must adopt specialized approaches to effectively

teach chemistry tailored to other disciplines. This essay explores the significance of teaching chemistry to non-chemistry students, the challenges involved, and effective pedagogical strategies that foster interdisciplinary learning. In my own experience there has been quite a lot of learning in teaching chemistry to non-chemistry students, especially to biologists and engineers.

# Why Chemistry Matters Everywhere

*From biology to engineering, **chemistry** is the foundation that connects innovation across disciplines.*



## 2. Importance of Teaching Chemistry to Non-Chemistry Majors

Teaching chemistry to students in other disciplines is not merely about transmitting facts; it serves a broader purpose of cultivating scientific literacy and critical thinking.

For example, a biologist with knowledge of chemical bonding and molecular interactions can better appreciate protein structure and function. An environmental scientist familiar with chemical equilibria can assess pollutant behavior in ecosystems more accurately. Engineers who understand chemical thermodynamics are equipped to optimize industrial processes for energy efficiency and safety. As the semiconductor sector attracts worldwide focus, chemistry major plays a key role in understanding and optimizing the molecular properties used in chip production.

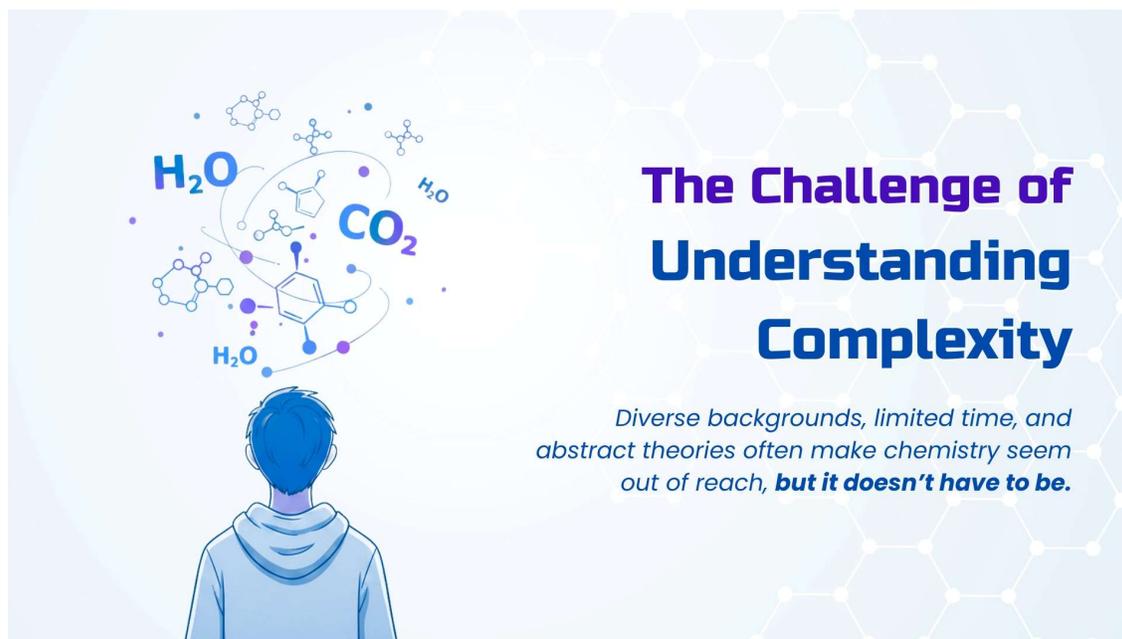
Moreover, interdisciplinary education fosters creativity and problem-solving skills by encouraging students to integrate knowledge from multiple fields. Real-world problems are

rarely confined to one discipline, and chemistry often provides the foundational language and concepts needed to address complex challenges such as climate change, drug development, or sustainable manufacturing.

## 3. Challenges in Teaching Chemistry for Other Disciplines

Despite its importance, teaching chemistry to non-chemistry students presents unique challenges. One of the most significant is the diversity in students' prior knowledge and motivation. Non-chemistry majors may have minimal exposure to foundational science and mathematics, making abstract chemical theories difficult to grasp. The symbolic language of chemistry—such as formulas, equations, and nomenclature—can appear intimidating and overly technical.

Students may also question the relevance of detailed chemical content, especially if it seems disconnected from their primary field of study. This perceived irrelevance can lead



to disengagement and poor performance. Additionally, time constraints in non-chemistry programs often limit how much chemistry can be covered, requiring educators to carefully select content without sacrificing essential understanding.

#### 4. Pedagogical Approaches and Strategies

Addressing these challenges demands innovative and student-centered teaching strategies. One effective approach is contextualization—teaching chemistry concepts through examples and applications directly related to students' disciplines. For biology students, linking chemical reactions to metabolic pathways or DNA structure helps clarify abstract concepts. Environmental science students benefit from studying chemical cycles and pollutant chemistry, while engineering students grasp material properties through case studies of alloys or polymers.

Active learning techniques enhance engagement and comprehension. Hands-on experiments, laboratory simulations, and virtual labs allow students to visualize and manipulate chemical phenomena, bridging theory and practice. Technology tools such as molecular modeling software or interactive quizzes provide immediate feedback and reinforce learning.

Collaborative learning and interdisciplinary projects encourage students to apply chemistry knowledge in real-world contexts, promoting deeper understanding and teamwork skills. For instance, joint projects between chemistry and environmental science students on water quality assessment integrate theoretical knowledge with practical investigation.

Supplementary tutoring, study groups, and online resources help students overcome initial difficulties and build confidence.

# Innovative Teaching, Inspired Learning

*Contextual, interactive, and technology-driven methods make chemistry engaging for every discipline.*



## 5. Curriculum Design and Content Selection

Effective chemistry teaching for other disciplines requires careful curriculum design that prioritizes core concepts relevant to students' fields. Essential topics often include atomic structure, chemical bonding, stoichiometry, thermodynamics, acids and bases, and reaction kinetics, but presented with an applied focus.

Modular curricula offer flexibility, allowing students or departments to select units most applicable to their goals. For example, medical students might focus on organic and biochemical chemistry, while for engineering students the emphasis may be on materials and physical chemistry.

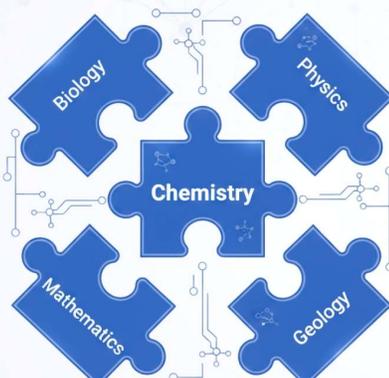
Integrating applied examples and case studies throughout the curriculum reinforces relevance and helps students connect theory to practice. Assessment methods should also align with learning objectives, incorporating practical problem-solving, interdisciplinary

case analysis, and project-based evaluations rather than solely traditional exams.

## 6. Role of Educators and Institutional Support

The success of teaching chemistry to other disciplines depends heavily on educators' expertise and institutional support. Educators must be trained not only in chemistry but also in interdisciplinary teaching methods and the specific needs of other disciplines. Institutions can facilitate collaboration between departments to develop integrated courses and share resources. Providing adequate laboratory facilities, technology tools, and teaching assistants enhances learning experiences. Partnerships with industry and research centers offer real-world perspectives and internship opportunities, motivating students and enriching curricula.

Continuous professional development and participation in chemistry education research enable educators to adopt best practices and innovate teaching methods.



## Designing for Relevance

*Flexible, modular curriculum built around chemistry concepts that align with each field's real-world needs.*

## Guided by Educators, Empowered by Institutions

*Collaboration, training, and resources form the backbone of **effective interdisciplinary teaching.***



### 7. Future Perspectives

Looking ahead, interdisciplinary science education is poised to grow in importance as global challenges become more complex. Digital tools and virtual laboratories will play

an increasing role in making chemistry accessible and engaging to diverse learners, overcoming geographic and resource limitations.



## Shaping the Future of Science Education

*Technology, flexibility, and  
collaboration will redefine how  
chemistry connects with every field.*

There is a growing emphasis on developing competencies such as critical thinking, problem-solving, and communication alongside content knowledge. Chemistry education tailored for other disciplines must adapt to these trends by embracing flexibility, technology integration, and collaboration.

Research into effective teaching practices and curriculum design will continue to inform improvements, ensuring that chemistry remains a vital component of multidisciplinary education.

### 8. Conclusion

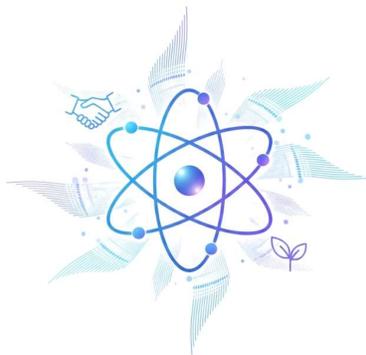
Teaching chemistry to students from other disciplines is essential for building a scientifically literate workforce capable of addressing complex, real-world problems. While challenges exist due to diverse backgrounds, motivation, and curriculum

constraints, adopting contextualized, active, and interdisciplinary teaching methods can greatly enhance learning outcomes. Educators and institutions must collaborate to design relevant curricula, support educators, and leverage technology to create engaging learning environments. Ultimately, effective chemistry education across disciplines fosters innovation, critical thinking, and collaboration that benefit science and society as a whole.

It's very apt at this era of industrial revolution to quote Prof. Ramsay's words: **"The country which is in advance of the rest of the world in chemistry will also be foremost in wealth and in general prosperity."**

— *William Ramsay (Nobel Prize in Chemistry, 1904)*

## Building a Scientifically Literate Future



*Chemistry empowers innovation, critical thinking, and collaboration,  
**the pillars of modern progress.***

## ABOUT THE AUTHOR



Dr. Sivapriya Kirubakaran is Professor in the Department of Chemistry and serves as Kankuben Bakshirambhai Gelot Chair at IIT Gandhinagar, Gujarat. Dr. Kirubakaran pursued her Ph.D. in Organic chemistry from Indian Institute of Science, Bangalore in 2007 under the guidance of Prof. S. Chandrasekaran. Following this, she did her postdoctoral studies from Harvard Medical School and Whitehead Institute, MIT on the chemical biology of kinases for cancer therapeutics. She is an experienced researcher and teacher with 20 years of experience in Organic chemistry and targeted drug discovery. Her current areas of interest include targeted drug discovery and medicinal chemistry. Her lab focuses on studying mechanistic pathways of DDR kinases using small molecules to develop novel therapeutics and exploring *Helicobacter pylori* survival pathways for developing drugs against the infection. Her long-term goal would be to make affordable medicines for cancer. Her work has yielded more than 60 publications and about 20 patents, wherein 6 Indian and 2 US patent have been granted. She is not only an acclaimed researcher but also a recipient of several awards including the alumni excellence award from The Ethiraj College for Women, 2024 and Dr. R. Gopalan Endowment prize (2022). In addition, she is a BIG-BIRAC grant awardee and a Ramanujan fellow (2013-2018). She is currently a CRSI council member and has been nominated as a member for “Future leaders” in the area of chemical biology by the Royal Society of Chemistry since 2023. She is featured in the book “India’s Science Geniuses” as one of the top 25 scientists from India. She recently founded and the chairperson of Procyll Therapeutics, a startup providing innovative solutions for effective drug discovery.

# Artificial Intelligence in Chemistry: Current Trends and Perspectives

Agastya P. Bhati

Wadhvani School of Data Science and Artificial Intelligence, Indian Institute of Technology (IIT)  
Madras, Chennai, Tamil Nadu, India 600 036

\*Email: agastya.bhati@dsai.iitm.ac.in

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**Artificial Intelligence (AI) is a powerful new technology that has gained a lot of traction in the past decade or so. It has found applications in almost every domain of our lives. Chemistry is no exception with an increasingly higher number of applications of AI in both basic and applied research. This has primarily been enabled by rapid accumulation of large datasets, accurate predictions of molecular properties, and automated experimental workflows. Advances in machine learning, deep learning, and data-driven modeling as well as computer hardware have led to major breakthroughs in drug discovery, materials science, spectroscopy, catalysis, and chemical education. In this article, I provide an overview of the various applications of AI in chemistry, emphasizing basic theoretical foundations, mathematical principles and exemplar use cases. By integrating chemical intuition and knowledge with data-driven approaches, AI is poised to become an essential component of modern chemical research.**

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## 1. Introduction

Chemistry aims to explain, anticipate, and manipulate matter on both the molecular and atomic scales. Traditionally, this knowledge comes from a mix of hands-on experiments, theoretical frameworks, and computer-based simulations. But with today's chemical research producing vast amounts of data from high-throughput testing, spectroscopy, quantum calculations, and materials databases, conventional methods can struggle to analyze everything efficiently.

Artificial Intelligence (AI) brings a fresh perspective by learning from data itself, instead of depending only on established physical theories. Within chemistry, AI is particularly effective at spotting trends in large, complex datasets and using these findings to predict chemical properties and

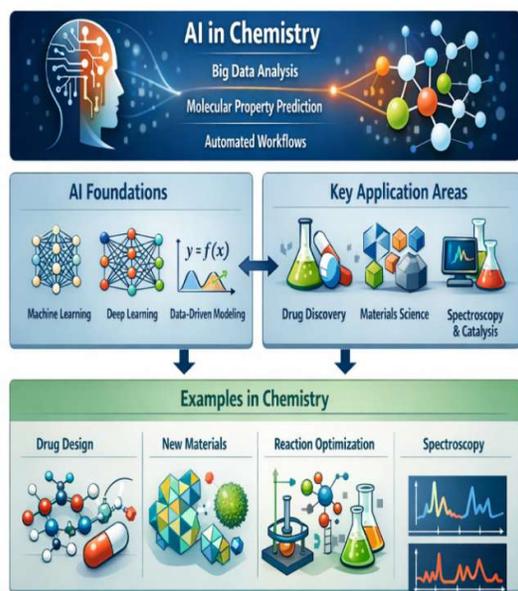
behaviors. Rather than replacing core chemical concepts, AI complements them—delivering quick estimates and assisting in planning experiments.

For undergraduates, AI opens new approaches to tackling chemical challenges by blending chemistry with math, statistics, and computing skills. Getting familiar with AI tools early helps students thrive in research where data-driven strategies are becoming standard.

## 2. Mathematical and Theoretical Foundations of AI in Chemistry

### 2.1 Chemical Data Representation

One of the main difficulties in using AI for chemistry is converting chemical information



**Figure 1:** A schematic providing an overview of the applications and utility of AI in the field of Chemistry. The readers should note that this image has been generated by AI (ChatGPT) providing the abstract of this article as the "prompt".

into numerical data that algorithms can interpret. Unlike text or images, molecules are three-dimensional, discrete, and influenced by quantum mechanics. To tackle this, various representation methods have been created. **Molecular descriptors** use numbers—like molecular weight, polar surface area, or electronegativity indexes—to capture key chemical characteristics, drawing on ideas known from physical and organic chemistry. **Molecular fingerprints** indicate whether certain substructures exist within a molecule, which helps with finding similar compounds or classifying them. However, these fingerprints can sometimes miss out on capturing all the detailed structural aspects. **Graph-based representations** model molecules as mathematical graphs, where atoms serve as nodes and bonds as edges. This approach closely matches chemical bonding theory and has gained popularity, especially

with the development of graph neural networks.

## 2.2 Machine Learning Paradigms

Supervised machine learning involves training models using labelled datasets made up of input–output pairs. In chemistry, inputs usually are molecular representations, and outputs can be physical, chemical, or biological properties. Mathematically, this approach seeks to approximate a function:

$$y = f(x)$$

Here,  $x$  denotes molecular features, while  $y$  represents a property of interest. A straightforward example is linear regression:

$$y = \alpha + \beta x$$

Although linear models are easy to interpret and apply, chemical relationships tend to be nonlinear. Therefore, flexible models like random forests and kernel-based methods are often preferred. Further, supervised learning plays a critical role in predictive modeling within chemistry. For example, by mapping molecular descriptors (features that numerically represent molecules, such as atom counts, ring structures, or quantum-chemical properties) to outcomes like solubility, toxicity, or reaction yield, researchers can accelerate material discovery and design new compounds with desired characteristics. Classification algorithms—such as support vector machines or neural networks—are often employed when the target property is categorical, like distinguishing between active and inactive drug candidates.

On the other hand, unsupervised learning methods, including clustering and dimensionality reduction, enable chemists to examine large data sets, identify patterns, and visualize chemical space— all without relying

on labelled data. They allow for the exploration of complex datasets where explicit labels are unavailable or difficult to obtain. Techniques such as hierarchical clustering or t-distributed stochastic neighbor embedding (t-SNE) help reveal natural groupings among molecules, which can suggest novel classes of compounds or highlight structure-activity relationships. Dimensionality reduction techniques like principal component analysis (PCA) are invaluable for visualizing high-dimensional chemical data in two or three dimensions, making it easier to interpret trends and outliers within vast chemical libraries.

In addition to supervised and unsupervised learning, semi-supervised and reinforcement learning approaches are emerging in chemical research. Semi-supervised learning leverages both labelled and unlabelled data, making it especially useful in domains where labelling is costly or time-consuming. Reinforcement learning, though less common, has found applications in automated synthesis planning and molecular optimization, where an agent learns optimal actions through trial and error to maximize a reward signal, such as synthetic feasibility or predicted biological activity.

By integrating these diverse machine learning paradigms, chemists are increasingly able to gain insights from large-scale datasets, model complex phenomena, and expedite the discovery and development of novel chemicals and materials.

### 2.3 Neural Networks and Deep Learning

Artificial neural networks are made up of layers of connected neurons, each performing weighted calculations and nonlinear

transformations on input data. Intuitively, neural networks draw inspiration from the human brain's architecture, with artificial neurons organized into layers—input, hidden, and output. As data passes through these layers, the network extracts increasingly abstract features, enabling it to tackle complex tasks such as image recognition, speech processing, and natural language understanding. The depth and flexibility of modern networks allow for remarkable performance across diverse fields.

Deep learning models feature multiple stacked layers, enabling them to learn complex, layered patterns. In chemistry, graph neural networks (GNNs) play a key role. They spread information through molecular graphs, allowing these models to understand how different atomic surroundings can affect the properties of molecules. For instance, GNNs enable accurate prediction of molecular properties, reactivity, or potential toxicity by learning from large datasets of known compounds. This approach has accelerated drug discovery and materials science, offering a powerful tool to model and predict the behaviour of unseen chemical entities.

Moreover, deep neural networks such as convolutional neural networks (CNNs) are widely used for analyzing images and spatial data, while recurrent neural networks (RNNs) are well-suited for sequential information, like time series or language data. These architectures have catalyzed advances in areas ranging from self-driving cars to automated translation.

### 3. AI in Molecular Property Prediction

Accurate prediction of molecular properties is a cornerstone of chemistry, influencing molecular behavior in chemical reactions, biological processes, and material applications. These properties—such as solubility, reactivity, toxicity, and spectroscopic signatures—help researchers design new molecules for drugs, materials, and catalysts. Conventional techniques typically depend on laboratory experiments or quantum chemical computations, both of which can be resource-intensive and time-consuming. For example, quantum mechanical calculations, like Density Functional Theory, may require hours or days to predict properties for moderately sized molecules, while experimental characterization involves synthesis, purification, and testing, consuming significant resources.

AI models offer an alternative by learning structure–property relationships directly from data, eliminating the need for explicit physical calculations. Machine learning algorithms, including deep neural networks, kernel methods, and decision trees, are trained on large datasets containing known molecular structures and their experimentally measured or calculated properties. Following training, these models can make predictions rapidly, thereby facilitating large-scale virtual screening efforts. This enables researchers to screen vast molecular libraries—sometimes millions of compounds—*in silico* before selecting promising candidates for further study, significantly reducing costs and accelerating discovery pipelines.

### Exemplars from Quantum Chemistry

Quantum chemistry relies on solving the Schrödinger equation. While these methods provide high accuracy, their computational cost increases significantly with system size due to the exponential scaling of electronic interactions. For instance, calculating properties for larger biomolecules or complex materials often becomes infeasible using traditional quantum chemistry techniques. In contrast, AI models empirically map molecular structures to properties, providing enhanced efficiency but sometimes sacrificing interpretability. The internal reasoning process of deep models may appear as a “black box,” making it difficult to extract mechanistic insights or guarantee generalizability beyond the training data.

This balance between speed and transparency positions AI as a valuable tool for exploratory research and preliminary screening, where approximate results are sufficient. However, for critical applications demanding high accuracy and mechanistic understanding, quantum chemistry remains indispensable. Integrating AI with quantum chemical approaches—through hybrid workflows or transfer learning—may harness the strengths of both paradigms, leading to more robust, interpretable, and efficient solutions in molecular science.

### 4. AI in Drug Discovery and Medicinal Chemistry

Drug discovery is a multidisciplinary endeavour that encompasses chemistry and biology. Given the vastness of chemical space, experimental approaches alone are insufficient, thereby necessitating AI solutions to efficiently prioritize promising

molecular candidates. AI technologies are integrated at various stages of drug development, including hit identification, lead optimization, and toxicity prediction. Leveraging historical datasets, AI models enable rapid evaluation of millions of compounds prior to laboratory synthesis.

One striking example of AI's impact can be seen in the identification of new antibiotics and antiviral compounds, where algorithms have rapidly sifted through chemical libraries to highlight candidates with unique scaffolds. However, despite these advances, challenges remain—data quality, model interpretability, and integration with wet-lab workflows pose ongoing hurdles. As computational power increases and data-sharing protocols improve, the synergy between experimental sciences and AI is anticipated to drive further innovation in pharmaceutical research.

#### **4.1 Virtual Screening and Binding Affinity Prediction**

Artificial intelligence models are employed to estimate binding affinity (defined as the change in free energy associated with the process of binding of a drug molecule to its target protein). These computational predictions assist researchers in selecting compounds with a higher likelihood of experimental success. Recent advances include the application of deep learning architectures such as graph neural networks and transformer-based models, which can capture subtle chemical features and interaction patterns. These models, when combined with high-throughput docking (less accurate but cheap) calculations, offer more accurate prioritization of candidate molecules. Future developments involve integrating structural data from cryo-EM or

advanced molecular dynamics simulations (more accurate but relatively more compute intensive), ultimately refining predictive accuracy and accelerating the cycle of hypothesis generation and testing.

#### **4.2 Generative Molecular Design**

Generative models facilitate the creation of novel molecules tailored to specific properties. This advancement transitions AI from a primarily predictive function to an innovative design tool, significantly expanding the toolkit available for medicinal chemistry. For instance, generative adversarial networks (GANs) and reinforcement learning frameworks now allow for the autonomous exploration of previously unseen regions of chemical space. These tools not only produce viable drug-like molecules but can also be optimized for multiple objectives simultaneously, such as potency, safety, and bioavailability. Looking forward, the refinement of generative models promises to reduce time-to-lead discoveries, minimize attrition rates during development, and enhance the overall efficiency of bringing new therapeutics to market.

### **5. AI in Materials Science, Catalysis, and Green Chemistry**

Materials science focuses on the discovery and development of substances with specific properties, such as electrical conductivity, mechanical strength, or catalytic efficiency. AI models facilitate this process by identifying relationships between material composition, structure, and performance, thereby allowing for efficient screening of potential candidates. For example, machine learning algorithms can predict the properties of untested materials,

reducing the need for time-consuming and costly laboratory synthesis. This accelerates the search for advanced materials used in technologies like batteries, solar cells, and flexible electronics. Additionally, AI-driven design platforms can suggest novel compounds based on targeted functionalities, broadening the scope for innovation.

In the field of catalysis, AI contributes to the optimization of active sites and reaction parameters through the analysis of experimental data sets. Machine learning tools assist chemists in determining the optimal conditions for catalytic reactions, such as temperature, pressure, and concentration of reagents, improving reaction yields and selectivity. AI has also enabled the rapid identification of new catalyst compositions that are more efficient or selective than traditional options.

Within green chemistry, AI advances sustainability objectives by uncovering energy-efficient processes and environmentally friendly reagents. For instance, AI can help identify solvent-free reaction pathways or propose alternative synthetic routes that generate less waste. By integrating predictive modeling with life cycle assessments, AI tools aid chemists and engineers in designing processes with a reduced environmental footprint, supporting the broader goals of sustainable development and responsible resource management.

## 6. AI in Analytical Chemistry

Spectroscopic techniques, widely used in analytical chemistry, produce data as intricate and multifaceted signals. These complex patterns are often difficult for human analysts to interpret accurately and

efficiently, particularly as the volume of data increases with high-throughput experimentation. AI has demonstrated exceptional ability in recognizing, extracting, and deciphering subtle patterns embedded in such datasets. By leveraging advanced pattern recognition and machine learning algorithms, AI systems can automate the analysis of spectroscopic data, reducing the manual burden on researchers and enabling more rapid extraction of meaningful chemical information. This automation not only streamlines workflows in analytical laboratories but also increases confidence in the consistency of results, as the process becomes less reliant on subjective human interpretation. This reduces the potential for human error and subjective bias—challenges that frequently arise in traditional manual analysis. The use of AI ensures that results are not only more consistent but also more reliable across different experiments and operators. Moreover, AI systems can process and analyze large quantities of spectral data at a speed unattainable by human analysts, dramatically accelerating research and development timelines. The resulting gains in efficiency enable researchers to redirect their focus toward deeper scientific inquiry and innovation, informed by high-quality, reproducible data.

## 7. Challenges and Limitations

AI holds great potential, but it also encounters issues like biased data, difficulties in understanding how decisions are made (lack of interpretability or explainability), and too much dependence on its predictions (technically named "overfitting"). Important ethical factors include being transparent, ensuring results can be reproduced, and

deploying AI responsibly. It's vital to teach students how to thoughtfully assess AI-generated outputs.

In addition to these concerns, AI systems can sometimes perpetuate social or cultural biases that exist within the datasets used for training. For example, a hiring algorithm may unintentionally favor one demographic group over another if the underlying data reflects historical inequalities. The "black box" nature of many AI models makes it challenging for users to interpret why certain decisions are made, raising questions about accountability and trustworthiness. Moreover, excessive reliance on AI could diminish critical thinking skills or lead to automation bias, where individuals accept machine outputs without proper scrutiny.

Ethical deployment also requires ongoing monitoring and evaluation to mitigate unintended consequences. Organizations must establish clear guidelines for data privacy, user consent, and the responsible use of sensitive information. Educators play a crucial role in equipping students not only with technical skills but also with the ability to evaluate the fairness, transparency, and societal impact of AI technologies. By fostering an environment where AI is used ethically and reflectively, we can help ensure that advancements in artificial intelligence contribute positively to society as a whole.

## 8. Future Outlook

The landscape of chemistry is poised for transformation through increased collaboration between human chemists and artificial intelligence systems. As AI technologies become more widely available,

undergraduate curricula should adapt accordingly to equip students with the necessary skills for data-driven chemical research.

Looking ahead, the integration of AI in chemistry could lead to significant advancements in areas such as drug discovery, materials science, environmental monitoring and many more. Machine learning models may help chemists quickly analyze massive datasets, predict molecular properties, and design novel compounds that were previously beyond reach. These innovations have the potential to accelerate the pace of scientific breakthroughs while expanding the frontiers of chemical knowledge.

However, this transformation also brings important challenges. Chemists will need to develop not only technical expertise in traditional laboratory techniques but also proficiency in digital tools, programming, and data analytics. Ethical considerations about AI's role in decision-making processes, responsible use of algorithms, and equitable access to these new technologies must also be addressed. By fostering interdisciplinary training and encouraging ongoing dialogue between chemists, computer scientists, and ethicists, the future of chemistry can harness the strengths of both human creativity and artificial intelligence.

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## ABOUT THE AUTHOR



Dr. Agastya P Bhati (Assistant Professor, Wadhvani School of Data Science and AI, IIT Madras) is a computational scientist with extensive experience in the field of computational biomedicine employing cutting-edge scientific methods including those based on artificial intelligence (AI). During his short career, he has published 26 papers across most high-profile journals and is well cited (over 1040 citations and *h*-index of 17). He has an extensive experience of performing large-scale simulations on various (pre)exascale supercomputers across the globe. He is currently leading the development of a novel computational workflow (IMPECCABLE) that combines physics-based methods with those based on AI to accelerate the process of drug discovery by coupling the two in an interactive and iterative way. IMPECCABLE aims at covering all aspects of early-stage drug discovery by not just identifying potent molecules but also optimising other properties such as toxicity and synthesisability. Further, he is active in the development of human digital twins for the advancement of healthcare, making it personalised and predictive.

## Crossword

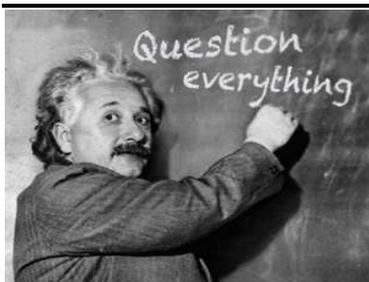
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**Across**

- 1 From the frying pan to Manhattan, it is quite slippery. (6)
- 5,16 A chilling blend that taught us how not do science. (4,6)
- 8 Vienna without me and an article is a great way to represent syllogism. (4)
- 9 To be or not to be falsified; that is the question to be a scientific theory. Thus spake \_\_\_\_\_ (6)
- 11 Abbreviated emergency room barely rusting helped grow the cutlery industry. (8)
- 12 Broken thermometer gives this dye from the Indian planation. (6)
- 14 The Greek astrological sign of Aries say they found lazy gases. (6)
- 17 This Deputy Commissioner of Police can extinguish many classes of fires. (3)
- 20 Howler somehow served a death knell for vitalism. (6)
- 23 Why you replaced in crystal – oh I see, to get the thin shell on the outside of the earth. (7)
- 24 It is a mixed-up deal, which will melt at 327° C. (4)
- 25 A war far in the countryside makes the blood thin (8).
- 26 The English fast bowler of the 60s doubles up as the father of epidemiology. (4)
- 27 And somehow, I was hounded out for my quasi concept. (3)

**Down**

- 1 I was forced to change my room with Iodine. (9)
- 2 Your logic is unclear to me. (5)
- 3 New York and London in parts weave a lovely net. (5)
- 4 Bond prefers “Shaken but not stirred” but I like “Broken but not shattered”. (10)
- 5 Maybe you can find me in house number 112 in Mendeleev Villa and what I like is the bright sun in the middle.  
(12)
- 6 Some nuclear reactors use water that cannot be taken lightly. (5)
- 7 A chaotic great order makes for a seemingly weird path for Saturn. (10)
- 10 I am both a creator and destroyer; creator of Bond and a destroyer of bacteria. (7)
- 13 The Japanese scientist who made a polymer that has something in common with Zubin Mehta. (9)
- 15 Sachin together with his car is so sweet. (9)
- 18 He put a chocolate in his pocket, and pulled out a microwave oven. (5)
- 19 This logic is not casual. (6)
- 21 Double \_\_\_\_\_; a type of experiments where both your eyes do not work. (5)
- 22 Scattering an arm gets you to Stockholm. (5)



1. If you were to plot pressure versus time in your household LPG cylinder, what would the graph look like and why?



2. In emergency situations on aircrafts, oxygen masks are deployed. Obviously, aircrafts cannot carry large oxygen cylinders, as it would be an extra load. What then is the source of this oxygen?



Answers for these questions will be published in the subsequent issue of the journal.

We invite readers to send any interesting questions, preferably with answers, that every chemistry student should know. The editorial team will decide whether the question and answer are suitable for publication. If published, the author(s) will be acknowledged.

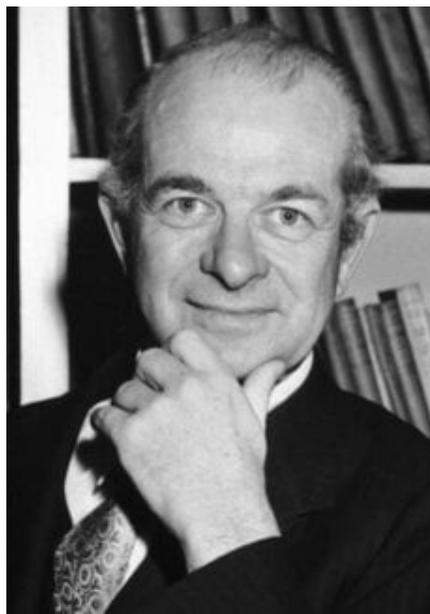
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## This Month in Chemical History

### 125 years of Pauling: A birthday launch for Kreative Chemistry Learning

As we launch the inaugural issue of the Kreative Chemistry Learning journal, we also celebrate the birthday of Linus Pauling, born on February 28<sup>th</sup>, 1901. His life's work serves as an example for the endless curiosity that this journal hopes to inspire, making it fitting that our first publication coincides with his birthday.

Pauling's profound contribution lies in how he redefined the rules of chemical bonding. He developed the first numerical scale of electronegativity, providing a framework to determine if a bond would be ionic or covalent. Furthermore, his introduction to concepts like orbital hybridization and molecular resonance made it possible to explain the stability and geometry of complex molecules that previous structures failed to capture. This earned him the Nobel Prize in Chemistry in 1954.



Beyond the laboratory, Pauling was an advocate for global peace and preservation of humanity. He leveraged his scientific platform to educate world leaders and the public about the biological dangers of radioactive fallout from above-ground nuclear testing. He was awarded the Nobel Peace Prize in 1962, making him the only person in history to receive two unshared Nobel Prizes.

Linus Pauling showed that chemistry is far more than equations; it is fundamental to different disciplines and a tool to advocate a safer and a better world. As we embark on our own journey of scientific exploration and communication with Kreative Chemistry Learning, Pauling's legacy stands as a guiding light and inspiration.

"If I have seen further, it is by standing on the shoulders of giants," - Sir Isaac Newton

Portrait of Linus Pauling obtained from:

<https://www.nobelprize.org/prizes/chemistry/1954/pauling/biographical/>



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