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CHEMSTREET

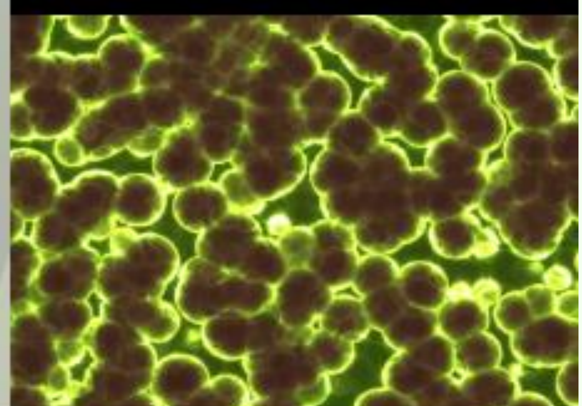
The Newsletter of Chemistry Department

Issue No. 5

Medical Microrobots

Rise of Machine

AI in Chemistry



Activities & Achievements

It Clicked! You See!

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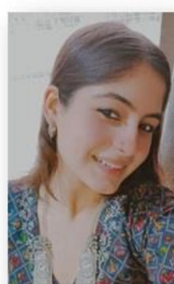

Ms. Unnati Makhija

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FROM EDITORS' DESK

Warm greetings to the readers of Newsletter!!

We are pleased to share with you the fifth issue of the Newsletter. In this edition, we are commemorating "AI and ML in chemical sciences". Scientifically speaking, computational chemistry in the present scenario provides a synergistic assembly between ab initio calculations, simulation, machine learning (ML) and optimization strategies for describing, solving and predicting chemical data and related phenomena. The AI and ML tools improve literature searches, analysis and prediction of physical and quantum chemical properties, searching transition states, chemical structures, chemical reactions, and also new catalysts and drug candidates.

The generalization of scalability to larger chemical problems, rather than specialization, is now the main principle for transforming chemical tasks in multiple fronts, for which systematic and economical solutions have benefited from ML approaches, including those based on deep learning (e.g., quantum chemistry, molecular screening, synthetic route design, catalysis, drug discovery). The ML algorithms tools corroborate with the raw input into layers of intermediate features, enabling bench-to-bytes designs capable of transforming a diversity of chemical domains. Multifarious chemical problems and respective rationalization, that were inaccessible because of unsuitable analysis tools, is thus detailed, evidencing the breadth of potential applications of these emerging multidimensional approaches. The models, algorithms and methods proposed facilitating research on fabrication of novel compounds, materials, forecasting the binding, molecular activity, and soft matter behavior are primarily focused. The information produced by pairing chemical sciences and ML, via data-driven analyses, neural network predictions and monitoring of chemical systems, allows (i) encouraging the ability to provide better insight into the intricacy of chemical information, (ii) rational design of the experiments, (ii) exploring novel molecular targets and materials, and also (iv) planning or revaluating upcoming chemical problems.

The current edition of "CHEMSTREET" newsletter provides an insight into the most inspiring developments concerning the use of ML in multifarious scenarios attributing to chemical sciences. Finally, we would also like to take this opportunity to thank the contributors of the newsletter for their constant support.

- Editorial Team

Message from Head of Department

Dear Colleagues and Students,

I am extremely delighted to share the 5th issue of our departmental newsletter. The present issue of "Artificial Intelligence" is particularly timely, as everyone seems to be talking about AI and with a good cause too. When it comes to Artificial Intelligence (AI), there are loads of opinions out in the field, like “AI is a fundamental risk to the existence of human civilization” by *Elon Musk*, “Strong AI would take off on its own and re-design itself at an ever-increasing rate. Humans, who’re limited by slow biological evolution, couldn’t compete and would be superseded” by *S. Hawkins*, and many more. Only time will tell which of the quotes on AI will predict the future reality closely. Its transformative impact can be seen in almost every sector. It’s become so general that we don’t realize we use it all the time, and it has found its way into our daily lives. Nowadays, AI and chemistry are inextricably linked, and we can see that their association has benefitted various fields of chemistry, like, Analytical Chemistry, Industrial Chemistry, Physical Chemistry, Energy Technology, Environment Chemistry, Biochemistry, Food, Agriculture, Materials Science, Inorganic Chemistry, Synthetic Chemistry, Organic Chemistry, Pharmacology, Toxicology, Pharmaceuticals, Natural products and many more. However, on analysing the trend in the implementation of AI in various sectors of chemistry, its popularity is reflected in the process of drug designing enormously. This edition highlights some of these associations. Finally, I wish all the best to the editorial team and contributors for bringing out the current issue of *CHEMSTREET*.

- **Prof. Rajib Bandyopadhyay**

Artificial Intelligence (AI) and Machine Learning (ML) Influencing Modern Chemical Science

-Dr. Prakash Chandra

Artificial intelligence (AI) addresses the potential of the machines to perform intelligently in giving decisions to novel inputs without accurately programming the same. The computer programs assist in the generation of outputs in accordance with the clear-cut commands, the AI predicts the outcome via data-fuelled models. AI in the time span of last two decades, advancements in AI and ML have revolutionized the approach of scientific research. AI and ML has recently contributed significantly in transforming the multifarious disciplines comprehending genome sequence mapping and exploration of novel antibiotics, influence of climate change on globe, delineating the existence of earth like planets in the galaxy.

Interestingly, chemical science is another domain, that has been untouched and has made huge leap after adopting AI and ML. AI finds applications in the multitudinous fields of chemical sciences to resolve the complicated relationship occurring between the present data sets. An interesting example for the application of AI in chemical science is prediction of solubility of the new compounds in accordance with the experimental data or theoretical predictions. AI has also proven beneficial in predicting the fate of organic reaction and seeking for suitable reaction conditions for optimize reaction yields. Alternative technique for the prediction of solubility of new compound based on the structure-solubility relationship after gaining experience on the solubility of know compounds. This white paper based on the "*Artificial Intelligence (AI) and Machine Learning (ML) Influencing Modern Chemical Science"* uncovers the linkage between AI and chemical science and mapping its influence on publication, patents and projects (PPPs). Moreover, this whitepaper also influences the future prospectus of the AI and ML yet to be unlocked has also been revealed.

How has AI and ML contributed to chemical sciences?

AI has largely been used in the chemical science research in drug discovery in reducing the cost of drugs and marketing out low cost and more efficient drug molecules in the market. In this context AI has made significant progress in drug discovery research and development. AI has accelerated drug discovery and reduce its huge costs and the time to market for new drugs.

However, the application of AI has not been limited to drug discovery. The AI and ML has also proven to be a valuable tool in predicting the mechanistic pathway of the chemical reaction via transition state search, optimizing the reaction conditions for improved substrate conversion and product yield. Furthermore, the AI and ML has been a value addition in the arsenal of the synthetic chemist's tool box in predicting the molecular properties, molecular design and retrosynthesis.

Predicting molecular properties

Whenever a synthetic chemist fabricates a new molecule for specific application, they employ complicated multistep synthetic pathway for the same. After the successfully synthesizing the molecules, they seek for appropriate properties suitable for desired application. However, in several cases the resulting molecules does not fulfil the criteria for desired application. Under these circumstances, the tedious synthetic steps are reinvestigated for the discovery of new molecule with all the desired properties, economical aspects, environmental aspects and toxicity. The repetitive process is time consuming and uneconomical.

Thanks to the modern AI and ML that ease the complication, time and money invested in the research of synthetic chemist by predicting the properties of hypothetical molecule and assisting the research to fabricate most promising molecules with all the desired properties. AI and ML provides Quantitative Structure-Activity Relationships (QSAR) or Quantitative Structure-Property Relationships (QSPR) as the important methods used for predicting the structure of molecules. The methods employ physical laws or phenomenological relationship assist in relating the properties of the molecules to the structural aspects. The ML algorithms assist in predicting the molecular solubility, boiling/melting point (BP/MP), toxicity, bioactivity, HOMO/LUMO molecular orbital theories, atomization energies and several other similar properties. AI algorithms are fed by multiple examples of several molecules and their relevant properties. Several regression or classification algorithms have been investigated for the linear regression, Support Vector Machines, Random Forests or Neural Networks. Algorithms associated with AI are suitable for resolving the problems based on the determination of molecular properties that are too complicated to establish. AI in corroboration with other prediction methods like physical laws or phenomenological relationship predict the relationship more accurately. Stacking provides interesting example is AI in corroboration with physical laws or phenomenological relationship as input data.

AI Facilitating Designing New Molecule

Fabrication of novel molecules is the most critical task for the synthetic chemist. Likewise, fabrication of novel complex organic molecules is only conceivable via the prior synthetic chemistry acquaintance and the inventiveness of the synthetic chemist. Furthermore, the molecular structure can be examined experimentally or in silico for anticipated outcome. The major restriction in the fabrication of novel molecules, that is, knowhow and predilection of the chemist to certain molecules, and may eliminate the fabrication of novel molecules that are beyond their scope. Another restraint can be the likelihood of fabricating novel molecular patterns that are impossible to virtually screen the synthetic strategy of these countless molecular structure in reasonable time. AI definitely augment the human intelligence via generating diversity of molecules in brief period of time. Several AL and ML based algorithms like variational autoencoders, adversarial autoencoders, recurrent neural networks and graph convolutional networks have recently emerged recently to resolve the human problem. These algorithms generate the molecular structures in form of SMILES strings or directly as graphical representation.

These algorithms generate molecular structures either as SMILES strings or directly as graphs, a more recent technique. These deep learning algorithms need to be trained on large numbers of molecules, typically millions, to construct a statistical distribution of the molecules. There is diversity of the training database available for free like ZINC database, the QM9 dataset of the ChEMBL database. Additionally, these algorithms assist in fabricating molecules owning the chemical miscellany as compared to those existing in the training database. The synthetic chemist can be trained to generate diversity of novel molecules by sampling the known statistical distribution close to molecule of interest. Moreover, instead of scanning diversity of molecules, the preference can be given to the limited number of more precise molecular structure with desired properties using Bayesian optimization technique to satisfy few desired properties.

Retrosynthesis

After singling out the appropriate molecule for possessing all appropriate properties its highly desirable to perform the retrosynthesis to map the commercially available starting materials in single or multistep synthesis. However, reterosynthesis is cumbering and synthetic chemist investa a major chunk of his time in this. Recently, computer-based programs have been used to assist the synthetic chemist, but these programs are of inferior quality and computer programs are of low quality as compared to those done by expert synthetic chemists. But, in the recent times, multiple high-performance ML-based algorithms have emerged as important research tools for synthetic chemists to assisting retrosynthesis. The complicated deep learning MLs trained on multimillions of organic reactions. The ML algorithm brings about a retrosynthesis tree composed of nodes (synthesis intermediate) and each leaf (commercially available starting material). These ML platforms are based on the corroborative effort of Monte Carlo tree search and deep learning algorithms. However, the major limitations to the current machine learning-based retrosynthesis algorithms are; (i) these are accurate for simple molecules but are not very effective for complex organic molecules like synthesis of natural products available in the literature; (ii) the training literature data sets are inaccurate and contain unreliable data, and the validity of these retrosynthesis routes are several times questionable; (iii) the algorithms are not reliable in predicting the sterochemistry of the product of reaction.

Conclusion

AI and ML tools in corroboration with the synthetic chemist's prior knowledge, skills assist in the fabrication of novel molecules design. In several cases, these synthetic chemists proved smart techniques provides impressive performance boosting synthetic chemistry. These AI and ML can be regarded valuable addition to the tool-box of the synthetic chemists to boost their laboratory skills with precision within limited time constrains. Moreover, AI-based retrosynthesis are significant tools for organic chemists via providing excellent starting points, and their results should be invested by experienced chemists prior to start synthesis in lab.

Click-See-Repeat: A Nobel Saga

-Dr. Nandini Mukherjee

Carolyn R. Bertozzi (Stanford University, USA); **Morten Meldal** (University of Copenhagen, Denmark), and **K. Barry Sharpless** (Scripps Research, La Jolla, CA, USA) won the Nobel Prize in Chemistry in 2022 "*for the development of click chemistry and bioorthogonal chemistry*." [1] The announcement must have been a moment of joy to organic chemists worldwide, especially those working at the interface of synthetic organic chemistry and biology.

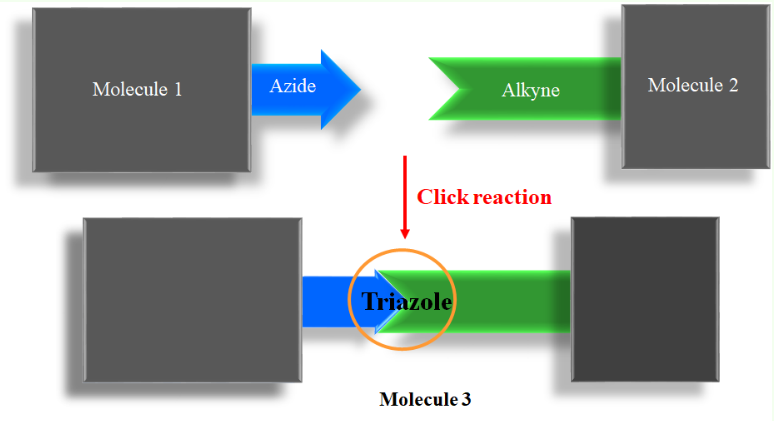
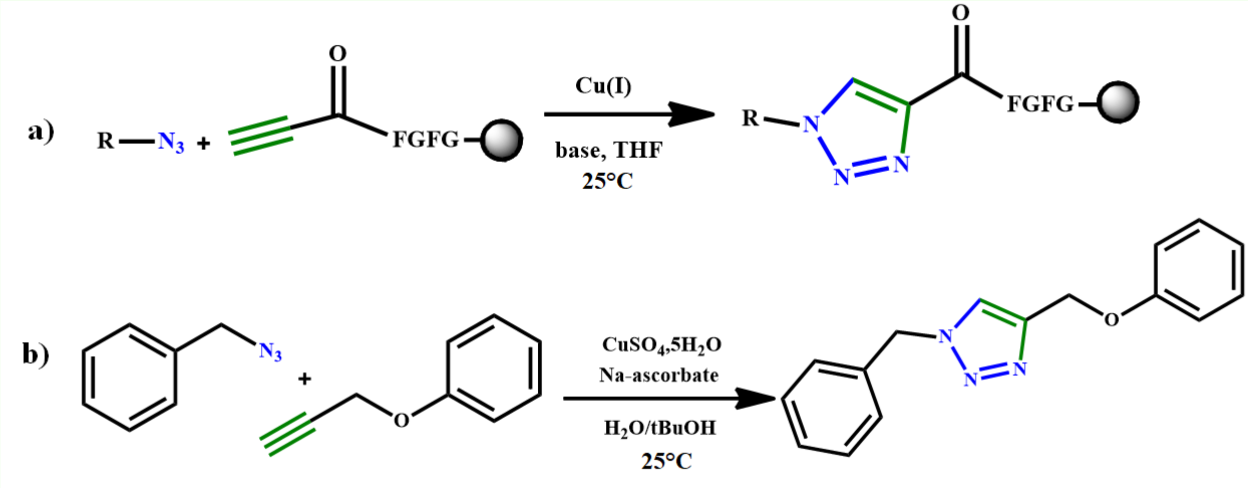


Figure 1. *Clicking of two small molecules to make a large molecule.*

'Click chemistry' a term aptly coined by Sharpless more than two decades ago, really means quick clicking or snapping of two molecules to form a larger molecule, with almost no byproduct formation. You might be wondering whether all molecules click with each other. Of course not! There has to be the presence of certain functional groups or modules in those two molecules. The most popular duo, which is almost synonymous with Click reaction now, is alkyne (C≡C) and azide (N_3) which post their "clicking" can form a triazole ring (see **Scheme 1**).



Scheme 1. *Copper-catalysed reactions from a) Meldal and coworkers [2] and b) Sharpless and coworkers; F: phenylalanine, G: glycine, filled circle: solid support, THF: tetrahydrofuran, tBuOH: tert-butanol [3,4].*

This reaction gives excellent yield when catalyzed with Cu(I) moiety. Morten Meldal enormously contributed to the copper-catalyzed azide-alkyne cycloaddition ("CuAAC" Click) reaction. Using different catalysts like Ru-complexes, you may get 1,5-disubstituted triazole, while the classical Cu(I)-catalyzed reaction yields 1,4-disubstituted triazole.

The reaction ticks off many of the criteria we look for in a successful synthetic route of any complicated large molecule: (a) Fast reaction with high yield; (b) negligible byproduct ensuring non-chromatographic separation process; (c) tolerance to a wide range of functional groups and therefore the wide scope of application; (d) can be done in mild condition even in the absence of solvent; (e) stereospecific; (f) insensitive to water and oxygen.

Large molecules can be made by the stepwise introduction of functional groups/fragments in a time-consuming, expensive, and elaborative process. But all synthetic chemists will tell you that no matter how much they like to explore new methodologies to make a compound, they want their reaction to succeed in the shortest timespan possible. There goes the cheer for Click chemistry. It's quick, easy, and simple! While we talk about Click reactions it would be an ungrateful act if we don't mention the pioneering contribution by **Arthur Michael** (1893),

Rolf Huisgen (1964) for the synthesis of 1,2,3-triazoles and the study of 1,3-dipolar cycloaddition respectively. In this context, it's worth noting that K Barry Sharpless has previously been awarded Nobel Prize in chemistry for the epoxidation reaction bearing his name (Sharpless epoxidation) and he is currently the only living chemist to bag two Nobels in chemistry.

Now, what click chemistry has to do with bioorthogonal chemistry? What is bioorthogonal chemistry by the way? Well, it means any chemical reaction that can occur inside a living cell (or body) without disrupting or being disrupted by the normal biochemistry of the cells. Carolyn Bertozzi coined the term 'bioorthogonal' and was the first scientist to apply Click reaction as a tool to study the living system as part of her cell surface engineering work. She made an azide-modified glycan (cell surface carbohydrate) to react with an alkyne-containing fluorescent molecule. Voila! The resultant triazole-derivative of previously dull, gloomy glycan, therefore, becomes fluorescent! You can now visualize and track the fluorescent glycan inside the cells! The illumination strategy can be applied to track other biomolecules too without killing the cells. This discovery brought a paradigm shift in live imaging and medicinal chemistry.

This work back then and its recognition now have inspired many of us! It will continue to inspire many of you. If you're one of our students attending an organic chemistry lecture/lab wondering what you will do with all the reaction schemes and mechanisms later, a Nobel Prize someday wouldn't be that bad, I suppose!

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Artificial Intelligence: Rise of the Machines

-Krunal Baria

Whenever the Artificial Intelligence (AI) word comes into the mind, most of the people think of AI named “J.A.R.V.I.S.” from the movie “Iron Man”. JARVIS is nothing but “Just A Really Very Intelligent System”. We all were captivated by how intelligent and cool the system was, which helped Tony Stark to make the “Iron Man” suits and later on helped him to find another core substance for his tiny palladium arc reactor.

Figure 1 JARVIS

We always wonder how just a computer program can be so reliable and trust worthy? To understand that we must look into past how the so called electrical smart machines, born from the contribution of inventions that make it so unusual.

The core need of any electrical machine is electricity. Benjamin Franklin, 1752 is given credit for discovering the electricity (the flow of electrons through a conductor). This electricity is used by the machine’s processor to perform the calculations. These calculations are made up with the use of transistors, that controls the flow of electricity by electrons zipping on and off as 1s and 0s.

“Silicon Valley” has dispensed cutting-edge technology in photolithographic techniques that are well accomplished in manufacturing huge integrated circuits called “chips” comprising of kilometers length of the conductors links up to 100 billion of transistor on numerous levels and have dimensions in a space no larger than a fingernail….!!!!

Figure 2 Central Processing unit

According to Moore's law, as the semi-conductor transistors gets smaller and smaller, the processing speed of a machine increases. Nonetheless, there should be a perimeter to the processing speed, and dimension limits of a transistor.

The contemporary companies like Intel are mass producing transistors 14 nanometer across. That is just 14 times wider than a DNA molecule. These transistors are made of Silicon, second most abundant material on the earth. Silicon's atomic size is 0.2 nanometer. Today's transistors are just 70 atoms of silicon wide. So, it is very challenging to make even smaller transistors. The transistors use electric signals in the form of electrons moving from one plane to another – to communicate. Scientist are finding ways to substitute electrons with light photons in order to obtain more speed at low energy.

Figure 3 IBM's 7nm transistors

Apart from the calculating system we need control system, an operating system is also an essential unit that con communicate with the machine's hardware. Operating system is all about the algorithms. Complex algorithms written in the form of codes to give commands and to perform calculations. The first operating system used for real work was the GM-NAA I/0, used by IBM 704 Main frame system in 1956. However, with the advancement in technology contemporaneous operating systems have become more sophisticated. The transition of these operating systems from the Command Line Interface (CLI) via Graphical User Interface (GUI) to Voice User Interface (VUI), it gets easier and easier to communicate with the machines.

Figure 4 What real coding looks like

Machines uses binary digit or bit 1 and 0 to store data and give commands. Binary 1 show that the transistor switch is on and binary 0 shows that the transistor switch is off. A single transistor is what called a BIT- binary digit. 8 of these bits makes 1 byte. Its noteworthy that today's computers use 32- or 64-bit system.

Figure 5 Inside a machine's mind

By setting a perfect algorithm we can train a machine to calculate certain types of functions and to store the data for the future use. The best real-life example is Google Alexa or Apple Siri. It's also made of complex algorithms written in the form of codes. The AI that can interact with the user verbally and can provide any data or perform any of the function. The same way we can also make our own JARVIS or Alexa. All you need is perfect hardware and very long complex codes for the desired algorithms. The application of AI in chemistry has been grown tremendously in this century. There were many AI related journal writing in the field of analytical and biochemistry.

With the growing technology we are giving more and more power to the machines, to make our life better than yesterday. In this day and age, machines are so ingenious and fast that they can see an object from a camera and can detect its color, temperature, inside frameworks etc. With the advancement in the technology, machines have become intelligent enough to acknowledge human voice and can also retort to it. The level in advancement is such that are capable of discerning more straightforward route for the destination via the application of GPS technology.

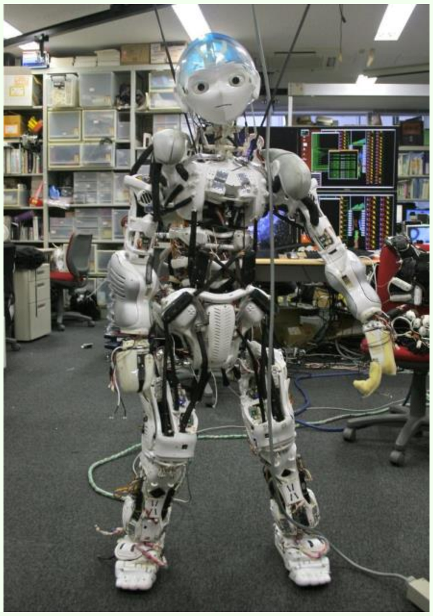

Figure 6: Kojiro Humanoid Robot, that can mimic the way skeleton, muscles and tendons works to generate motion

Nowadays, machines are so clever that they can outperform any human on the earth. But still, they don’t have one thing that a living creature can have and it is the Emotions. Emotions can’t be programmed and that’s the reason why machines are reliable and trustworthy, as they only follow the commands.

Medical Microrobots

-Jeny Gosai & Nikunj Vagadiya

One day, a visit to the hospital with a serious illness could end not with surgery or bottles of pills, but with an injection of medical microrobots. Similar in size to living human cells, microrobots are far less likely to cause tissue damage than conventional medical interventions, such as surgical incisions and catheter insertions. By aiming for specific destinations in the body, microrobots could drastically reduce the side effects of pharmaceuticals.

Figure 1: Poster of Fantastic voyage (1966)

In the 1966 film Fantastic Voyage, scientists shrink a submarine to smaller than a red blood cell and drive it through blood vessels en route to the brain in an attempt to remove a life-threatening clot. The fantastical notion of shrinking people to a few microns aside, the narrative was physics challenged in other ways. At such a small scale and in a fluid as thick as blood, the shrunken submarine's teeny propellers wouldn't be able to move the ship, for example.

Surgical procedures that could be performed by a microrobot include opening of clogged vessels or other channels, cauterization, treatment of hyperthermia, biopsies, electrical stimulation, injection, cutting, drilling, or biomaterial removal. Several groups to date have investigated the use of integrated biopsy tools for capsule endoscopes to collect tissue samples for diagnostic purposes. Expansion of these capabilities into surgical microrobots would enable more precise targeting of sampling locations using a minimally invasive surgical system. Others have proposed magnetic robots that could be used to puncture or open clogs in blood vessels. To date, only a limited number of studies on the use of microrobots for minimally invasive surgery have been undertaken. However, as methods for propulsion and control have improved, microrobots could find a broad range of potential applications throughout the human body.

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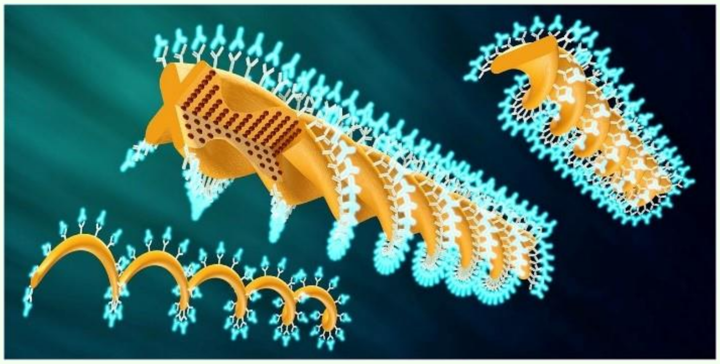

Figure 3: In 2014, researchers at eth zurich devised microrobots that propel themselves by twisting, something like an artificial flagellum. Researchers direct the microrobots with external magnetic fields.

Bradley Nelson, an engineer at ETH Zurich and his team introduced a T. brucei-inspired "origami robot," a self-folding micromachine, made from a hydrogel, that optimizes its shape according to the viscosity and temperature of its environment (1). It propels itself forward—in experiments, through a viscous sugar solution—by whipping a flagellum-like tail. Scientists steer it by manipulating external magnetic fields.

The researchers tested its capabilities via a simulated oesophagus and stomach, which had been 3D printed from silicone to match the structure and viscosity of the real thing. Using magnetic fields, the researchers navigated the unfolded robot into the stomach, where it attached to and removed a battery embedded in the lining.

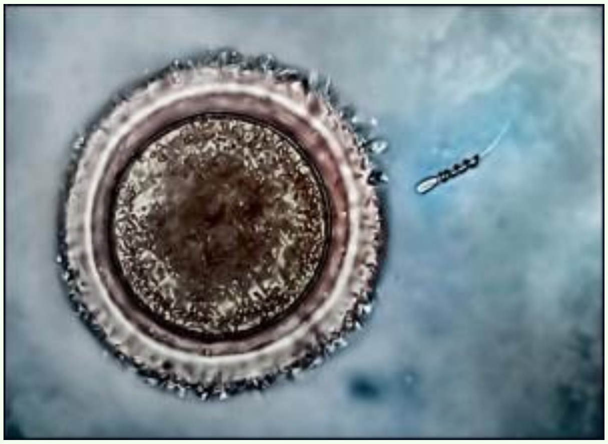

Figure 4: A helical micromotor helps an immotile but healthy bovine sperm cell get to an egg in culture.

In 2013, a group at the Institute for Integrative Nanosciences in Dresden, Germany, debuted a device that traps bull sperm in magnetic nanotubes and uses the cells for propulsion (5); magnetic fields are used to steer. Last year, the same group (6) unveiled a remote-controlled “spermbot,” which can fit on a slow sperm and escort it to an egg as a possible treatment for infertility.

In March 2017, robotics researchers at Tohoku University, in Japan, introduced an “amoeba-like” molecular robot made of natural molecules—including DNA, lipids, and proteins—that changes its shape in response to chemical and light cues.

Over the past 15 years the field of microbots has exploded with many teams from around the globe contributing to major innovations. A myriad of synthetic microbots, based on various propulsion mechanisms and different designs and materials, have thus been developed. New functionalities and capabilities have been added to these tiny machines, including fast motion in complex biological media, large cargo-towing force, collective behavior and excellent biocompatibility for use in living systems. These attractive capabilities have paved the way to sophisticated microscale robotic devices capable of performing complex tasks and have motivated researchers to explore exciting new important in vivo biomedical applications. Looking further ahead, once they can be manipulated accurately and repeatedly at the subcellular size range, microrobots could in near future enable tissue engineering and regenerative medicine, whereby damaged tissue and organs could be repaired or entirely rebuilt.

DEPARTMENTAL EVENTS & ACTIVITIES

Workshops/Webinars Organized

Nitin Chaudhari

Monthly webinar series organizer and coordinator for Chemistry Colloquium Series (CHEMTALKS) on 31/01/2022 and 23/02/2022.

Rama Gaur

Co-ordinated Popular Lectures on Science Day and Science Day Quiz on 27-28 Feb 2022.

Syed Shahabuddin

1. National webinar on strategies for scientific research publications at Government Degree College, Neeli Nallah, Udhampur, Jammu & Kashmir on 26th March 2022.

2. STTP: 5 day Hands-On Workshop on Synthesis of Nanomaterials and Nanocomposites 25 April–29 April 2022.

RESEARCH PUBLICATIONS

Anu Manhas

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2. K. Patil, P. Shinde, P. Srinivasappa, W. Nabgan, Nitin. K. Chaudhari, C. Rout, A. Jadhav, "Rational Competent Electrocatalytic Oxygen Evolution Reaction on Stable Tailored Ternary MoO3-NiO-Activated Carbon Hybrid Catalyst", International Journal of Energy Research, 2022. Early view (Impact Factor-5.2)

Prakash Chandra

1. Advanced Copper based Nanostructured Materials for Oxidative Methyl-esterification Reactions- a Mini Review (Accepted in Materials today, Proceedings).
2. Recent Trends in MXene/Metal Chalcogenides for Electro-/Photocatalytic Hydrogen Evolution Reactions (Accepted in International Journal of Hydrogen Energy doi.org/10.1016/j.ijhydene.2022.02.049).
3. Advanced MoS_2 nanocomposite materials for the synthesis of valuable pharmaceuticals R Gaur, N Mukherjee, S Shahabuddin, P Chandra Materials Today: Proceedings.
4. Conducting polymers-based nanocomposites: Innovative materials for waste water treatment and energy storage S Shahabuddin, R Gaur, N Mukherjee, P Chandra, R Khanam Materials Today: Proceedings.
5. Recent advances in nanostructured transition metal sulfide-based sensors for environmental applications R Gaur, S Shahabuddin, N Mukherjee, P Chandra Materials Today: Proceedings
6. Recent progress in lysosome-targetable fluorescent BODIPY probes for bioimaging applications N Mukherjee, R Gaur, S Shahabuddin, P Chandra Materials Today: Proceedings.
7. Hydrothermal synthesis of graphene modified SnO nanocomposite for oxygen reduction reaction S Soren, S Chakroborty, L Pradhan, P Chandra, J Sahu, P Parhi Materials Today: Proceedings.

Rajib Bandyopadhyay

Zeolite Y from kaolin clay of Kachchh, India: Synthesis, characterization and catalytic application, Journal of the Indian Chemical Society 98 (2021) 100246.

Rama Gaur

1. Rama Gaur*, Syed Shahabuddin, Nandini Mukherjee, Prakash Chandra, Recent advances in nanostructured transition metal sulfide based sensors for environmental applications, Materials Today: Proceedings, 2022, ISSN 2214-7853, https://doi.org/10.1016/j.matpr.2021.12.330.
2. Syed Shahabuddin, Rama Gaur, Nandini Mukherjee, Prakash Chandra, Rashmin Khanam, Conducting polymers-based nanocomposites: Innovative materials for waste water treatment

and energy storage, Materials Today: Proceedings, 2021, ISSN 2214-7853, https://doi.org/10.1016/j.matpr.2021.12.335

3. Nandini Mukherjee, Rama Gaur, Syed Shahabuddin, Prakash Chandra, Recent progress in lysosome-targetable fluorescent BODIPY probes for bioimaging applications, Materials Today: Proceedings, 2022, ISSN 2214-7853, https://doi.org/10.1016/j.matpr.2022.01.220

4. Rama Gaur, Nandini Mukherjee, Syed Shahabuddin, Prakash Chandra, Advanced MoS2 nanocomposite materials for the synthesis of valuable pharmaceuticals, Materials Today: Proceedings, 2022, ISSN 2214-7853, https://doi.org/10.1016/j.matpr.2021.12.372.

5. Krunal Parekh, Syed Shahabuddin, Rama Gaur, Niragi Dave, Prospects of conducting polymer as an adsorbent for used lubricant oil reclamation, Materials Today: Proceedings, 2022, ISSN 2214-7853, https://doi.org/10.1016/j.matpr.2022.01.130.

Proceedings in Materials (International Symposium on Materials of the Millennium: Emerging Trends and Future Prospects (MMETFP-2021))

6. Veena Sodha, Rama Gaur, Rajib Bandyopadhyay, Syed Shahabuddin, Zeolites based nano-composites for waste water treatment

7. Jinal Patel, Stuti Jha, Syed Shahabuddin, Rama Gaur* A Review: Carbon Based Materials for Photocatalytic Degradation of Agrochemicals

8. Stuti Jha, Jinal Patel, Syed Shahabuddin, Rama Gaur* Biochar: A Sustainable Approach towards Environmental Remediation.

9. Darban Zenab, Rama Gaur, Syed Shahabuddin, Hydrogel-based adsorbent materials for heavy metal removal from industrial waste water.

10. Rushik Radadiya, Syed Shahabuddin, Rama Gaur*, Waste to Best: Chemical recycling of polyethylene terephthalate (PET) for generation of useful molecules.

11. Krunal Parekh, Rama Gaur, and Syed Shahabuddin* , Recent Advances in Reclamation of Used Lubricant Oil.

12. Darban Z, Shahabuddin S, Gaur R, Ahmad I, Sridewi N. Hydrogel-Based Adsorbent Material for the Effective Removal of Heavy Metals from Wastewater: A Comprehensive Review. Gels. 2022 Apr 22;8(5):263.

Syed Shahabuddin

1. Michael FM, Khalid M, Chantara Thevy R, Raju G, Shahabuddin S, Walvekar R, Mubarak NM. Graphene/Nanohydroxyapatite hybrid reinforced polylactic acid nanocomposite for load-bearing applications. Polymer-Plastics Technology and Materials. 2022 May 24;61(8):803-15.

2. Thachnatharen N, Khalid M, Shahabuddin S, Anwar A, Sridewi N. Tribological analysis of advanced microwave synthesized Molybdenum disulfide (MoS2) as anti-friction additives in diesel engine oil for military vehicles. Materials Today: Proceedings. 2022 Apr 28.

3. Darban Z, Shahabuddin S, Gaur R, Ahmad I, Sridewi N. Hydrogel-Based Adsorbent Material for the Effective Removal of Heavy Metals from Wastewater: A Comprehensive Review. Gels. 2022 Apr 22;8(5):263.

4. Abdelnasir S, Mungroo MR, Shahabuddin S, Siddiqui R, Khan NA, Ahmad I, Anwar A. Polyaniline (PANI)-conjugated tungsten disulphide (WS2) nanoparticles as potential therapeutics against brain-eating amoebae. Applied Microbiology and Biotechnology. 2022 Apr;106(8):3279-91.

5. Shah SN, Shahabuddin S, Khalid M, Mohd Sabri MF, Mohd Salleh MF, Muhamad Sarih N, Rahman S. Rheological and Thermal Conductivity Study of Two-Dimensional Molybdenum Disulfide-Based Ethylene Glycol Nanofluids for Heat Transfer Applications. Nanomaterials. 2022 Mar 21;12(6):1021.

6. Alamgir M, Shahabuddin S, Mallick A, Nayak GC. Processing of pHEMA/TiO2 based nanocomposites used as an excellent dental materials. Materials Today: Proceedings. 2022 Feb 18.

7. Mansur FA, Sridewi N, Anwar A, Anwar A, Shahabuddin S. Polypyrrole-conjugated zinc oxide nanoparticle as antiamoebic drugs against Acanthamoeba castellanii. Materials Today: Proceedings. 2022 Feb 7.

8. Mukherjee N, Gaur R, Shahabuddin S, Chandra P. Recent progress in lysosome-targetable fluorescent BODIPY probes for bioimaging applications. Materials Today: Proceedings. 2022 Feb 2.

9. Parekh K, Shahabuddin S, Gaur R, Dave N. Prospects of conducting polymer as an adsorbent for used lubricant oil reclamation. Materials Today: Proceedings. 2022 Jan 31.

10. Gaur R, Shahabuddin S, Mukherjee N, Chandra P. Recent advances in nanostructured transition metal sulfide based sensors for environmental applications. Materials Today: Proceedings. 2022 Jan 8.

11. Gaur R, Mukherjee N, Shahabuddin S, Chandra P. Advanced MoS2 nanocomposite materials for the synthesis of valuable pharmaceuticals. Materials Today: Proceedings. 2022 Jan 5.

12. Shahabuddin S, Gaur R, Mukherjee N, Chandra P, Khanam R. Conducting polymers-based nanocomposites: Innovative materials for waste water treatment and energy storage. Materials Today: Proceedings. 2021 Dec 31.

13. Shahabuddin S, Baharin SN, Suhaimi NF, Yunus N, Sambasevam KP. Preparation of shrimp-based chitin blend with polyaniline for chromium (VI) removal from aqueous solution. Materials Today: Proceedings. 2021 Dec 30.

RESEARCH GRANT

Nitin Chaudhari

CENTRAL POWER RESEARCH INSTITUTE- BANGALORE, under Ministry of Power, GOI. Total Cost- 48.49 Lakhs for 2 years.

EXPERT TALK DELIVERED/ORAL PRESENTATION IN CONFERENCE-WEBINAR-SYMPOSIUM

Nandini Mukherjee

1. Oral presentation in the '1st International Conference on Advances in Water Treatment and Management' on 26th March, 2022 at PDEU, Gandhinagar.

2. Presented poster on ‘Anion detection employing synthetic chemosensors in aqueous media', ICAWTM 2022, Pandit Deendayal Energy University, mar 2022.

3. Presented poster at the "2nd Faculty Review Symposium" for School of Technology on 5th March, 2022 at PDEU, Gandhinagar.

Dr. Nitin Chaudhari

1. Dr. Nitin Chaudhari gave Invited Talk on "Recent Advances in Fuel Cell Technology and Electrochemical Hydrogen Production" at international conference on Global Trends in Science, Technology, Humanities, Commerce & Management (ICGTSTHCM 2022) on 2nd January 2022.

2. Dr. Nitin Chaudhari delivered a Keynote Invited Talk on "Recent Advances in Fuel Cell Technology and Electrochemical Hydrogen Production" at international conference on Global Trends in Science, Technology, Humanities, Commerce & Management (ICGTSTHCM 2022) on 2nd January 2022.

Prakash Chandra

1. The Top Techs Trending Now in Chemical Sciences "CHEMTALKS: A Chemistry Colloquium Series on 23rd February 2022"

Rama Gaur

1. Poster Presentation: “Facile synthesis of Type II ZnO-CdS nanostructures for applications in waste water treatment” at International Symposium on Materials of the Millennium: Emerging Trends and Future Prospects. Pandit Deendayal Energy University, Gandhinagar during 19-20 November 2021.

2. Presented a poster on "Waste to Best: A sustainable strategy for environmental remediation" #RSCPoster Twitter Conference - webinar series on 1st March 2022.

Syed Shahabuddin

1. An expert invited talk on STRATEGIES FOR SCIENTIFIC RESEARCH PUBLICATIONS at National webinar on strategies for scientific research publications at Government Degree College, Neeli Nallah, Udhampur, Jammu & Kashmir on 26th March 2022
2. An expert talk on Characterization Techniques for the analysis of synthesized nanoparticles at 5 days hands on workshop on synthesis of nanomaterials and nanocomposites from 25 April 29 April 2022 PDEU
3. An expert talk on Photocatalysis: An effective tool for degradation of organic pollutants at 5 days hands on workshop on synthesis of nanomaterials and nanocomposites from 25 April 29 April 2022 PDEU
4. An expert Hands on Session on photocatalysis on reactor using synthesized photocatalyst at 5 days hands on workshop on synthesis of nanomaterials and nanocomposites from 25 April 29 April 2022 PDEU.

PARTICIPATION IN FDP

Anu Manhas

5-day online FDP on the theme “Inculcating Universal Human Values in Technical Education” organized by All India Council for Technical Education (AICTE) from 27th December, 2021 to 31st December, 2021.

HONOURS/AWARDS/RECOGNITION

Nandini Mukherjee

1. Third prize for poster presentation at the "2nd Faculty Review Symposium" for School of Technology on 5th March, 2022 at PDEU, Gandhinagar.
2. Best Oral Presentation Award in the '1st International Conference on Advances in Water Treatment and Management' on 26th March, 2022 at PDEU, Gandhinagar.

Nitin Chaudhari

1. Dr. Nitin Chaudhari has been selected on the Editorial Board of Frontiers in Energy Research Journal as Review Editor for the Electrochemical Energy Conversion and Storage area, from December 2021.

Syed Shahabuddin

1. Selected as Review Editor on the Editorial Board of Electrochemical Energy Conversion and Storage: Frontiers in Energy Research.
2. Appointment as a Collaboration Partner for Collaborative Teaching Initiatives at UiTM Negeri Sembilan Branch (KUALA PILAH CAMPUS), Malaysia.

Student Corner

As a celebration of international women's day, Self-defence session was taken by Master Pragnesh Messariya, Ishita Parmar and Jeny Gosai at Rashtriya Raksha University on 8th March 2022.

Women’s day special session on self-defence by Master Pragnesh Messariya, Ishita Parmar and Jeny Gosai at Gandhinagar on 5th March 2022.

October 2022

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CHEMSTREET

"An expert is a person who has made all the mistakes that can be made in a very narrow field."
– Neils Bohr

Cover & Back Cover by Dr. Nandini Mukherjee