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Role of Nanoscience in Artificial Intelligence

Dr. Biplab Goswami

Department of Physics, Sreegopal Banerjee College, Mogra, Hooghly 712148, West Bengal, India
Email: *gwbiplab[at]gmail.com*

Abstract: ***Compound semiconductor nanocrystals (quantum dots) are exciting class of materials whose optical and electronic properties can be manipulated by changing their size or composition. Artificial intelligence (AI) is a wide - ranging branch of computer science concerned with building smart machines capable of performing tasks that typically require human intelligence. The goals of artificial intelligence include computer - enhanced learning, reasoning, and perception. AI is being used today across different industries from finance to healthcare. The Application of AI in Atomic Force Microscopy and SEM, Nanoscale Simulations and the relation between Artificial Intelligence and Nano - Computing are our interest of studies. Bridging the link between current nanosciences and AI can boost research in these disciplines and provide a new generation of information and communication technologies that will have a large impact in our society, probably providing the means so that technology and biology merge.***

Keywords: Nano particles, Quantum confinement effect, Artificial Inteliigence, Nano Technology, Nano - computing, Drug delivery.

1. Introduction

When Richard Feynman, an American Physicist and winner of Nobel prize and physics professor at California Institute Technology (CalTech), gave a talk under the title of *"There is Plenty of Room at the Bottom"* [1] at an American Physical Society (APS) meeting during December 29th, 1959, at CalTech, California, the door to ideas and concepts behind nanoscience and nanotechnology just got opened. Of course, this talk was way before the term 'nanotechnology' was used in our ordinary daily English language.

Advances in nanoscience and nanotechnology promise to have major implications for advances in the scientific field as well as peace for the upcoming decades. This will lead to dramatic changes in the way that material, medicine, surveillance, and sustainable energy technology are understood and created. Significant breakthroughs are expected in human organ engineering, assembly of atoms and molecules, and the emergence of a new era of physics and chemistry.

Mathematician Alan Turing changed history with a simple question: *"Can machines think?"* Turing's 1950 paper "Computing Machinery and Intelligence" [2] and its subsequent Turing established the fundamental goal and vision of AI.

AI is an approach to inculcate human - like thinking into an electronic gadget of any scale. This is an analysis of how human brain as it attempts to solve problems, thinks, learns, decides and works. It is heavily inspired by biological anatomy for the development of prevalent and most effective models, viz., artificial neural networks (ANNs) and other such algorithms [3]. An important AI goal is to improve machine functions related to human intelligence such as reasoning, thinking, and problem solving.

A combination of these two fields can result in great breakthroughs from the fast - paced AI assisted nanotechnology research [4 - 6] to creating the state - of - the - art materials, to expand the application area of AI using nanotechnology - based computing devices. Besides merging the two technologies, a combined research can also give a thrust to the study in each discipline, possibly leading to all sorts of new methods to gain insights and communication technologies.

1) Nanomaterials

Anytime, these days, when talking about nanomaterials, we should think about how small things can be, such as an atom of any element or from a scaling point of view, what would be the *"Size of the Nanoscale"* or basically, just how small is "nano?" and what can we imagine about the scale of from Microscopic perspective. From metric MKS unit dimensional point of view or International System Units (ISU), the prefix "nano" means one - billionth or 10^{-9}, therefore, one nanometer is one - billionth of a meter. The nanomaterials possess a variety of unique physical and chemical properties.

Nanoparticles and nanomaterials continue to attract a great deal of attention because of their potential impact on an incredibly wide range of industries and technologies [7 - 11]. In the nanometer regime, their fundamental properties depend on a unique parameter size. The rapid growth of research in this field is because of the fact that the structural, electronic, and optical properties of nanoparticles can be tuned by varying their size. These features arise from what is known as the quantum confinement effect or quantum size effect. When the crystal size becomes comparable with the Bohr radius, the result is quantum confinement, and the bandgap becomes size dependent. The sizedependent bandgap energies of semiconductor nanocrystal spanning has a remarkable spectral range from visible to near - infrared (IR), leading to their implementation as a fluorescent biological effect level, laser materials, and chromophores in light - emitting diodes (LED) [11 - 12]. The chemical properties, categories being electronic and optical are present in the form of bulks and are very distinctive of each other. When the materials are present in nano size, their properties are hard to identify as compared to the times when they are present in the larger size. Almost all the properties of nanoparticles are dependent upon their size [13 - 18]. One of the most remarkable properties of nanoparticles is their diffusion. They are extremely efficient and carry out the process of diffusion so well but it takes place only at high temperatures due to the high surface area to the volume ratio. The basic properties of these materials

are that they possess a definite shape with approximate fixed size, possess surface characteristics, and also have an inner structure.

Artificial Intelligence

Artificial intelligence (AI) is a vast emerging field that can be very thought provoking. AI has been seen recently in a number of movies and television shows that have predicted what the possibility of an advanced intelligence could do to our society. This intellect could possibly outperform human capabilities in practically every field from scientific research to social interactions [19 - 21]. Aspirations to surpass human capabilities include tennis, baseball, and other daily tasks demanding motion and common sense reasoning (Kurzweil, 2005). Examples where AI could be seen include chess playing, theorem proving, face and speech recognition, and natural language understanding. AI has been an active and dynamic field of research and development since its establishment in 1956 at the Dartmouth Conference in the United States (Cantu - Ortiz, 2014). In past decades, this has led to the development of smart systems, including phones, laptops, medical instruments and navigation software [22].

In simple terms, AIs can help us to understand the ways in which materials work at the nanoscale. This might allow us to build computers at this scale that are not dependent on the transistor - based architecture that most computers today are based on. This, in turn, will allow the creation of ever more sophisticated AIs, which will allow us to probe this behavior still further. In the same way that neural networks could help computers code themselves, nanocomputing technologies could allow computers to build themselves.

Psychology and Neurosciences have helped to comprehend brain - functionality and lessened the gap between humans and mystery of consciousness [23]. This consequently gave origin to exploring and creating AI and there is much work to be done. Artificial intelligence is an attempt to replicate human intelligence with the help of machines by using resources governed by data science and machine learning. Efforts are being put in by researchers to make the machine mimic cognitive abilities possessed by humans among many capabilities. Some of the common daily use of the AI can be seen in Apple's assistant "Siri", Google's assistant, Microsoft's assistant "Cortana" and Amazon's assistant "Alexa". Tesla has managed to put a self - driving car using artificial intelligence. Above examples show how AI has managed to improve comfort levels for humans by allowing to converse with your mobile device or home assistant device to play music or to relax and not worry about driving. It must be noted that there are some aspects of use of AI which are controversial from ethical stand point and therefore under scrutiny.

Technology that operates on the nanometre scale often involves intricate systems that are not always suited to the various facets of AI. However, there are some growing areas where AI converges with nanotechnology. In addition to merging the two technologies, combined work in nanotechnology and AI can also boost study in each discipline, possibly leading to all kinds of new tools for gaining insights and communication technologies.

Types of AI

Artificial intelligence can be categorized into four types:

a) **Reactive AI** uses algorithms to optimize outputs based on a set of inputs. Chess - playing AIs, for example, are reactive systems that optimize the best strategy to win the game. Reactive AI tends to be fairly static, unable to learn or adapt to novel situations. Thus, it will produce the same output given identical inputs.
b) **Limited memory AI** can adapt to past experience or update itself based on new observations or data. Often, the amount of updating is limited (hence the name), and the length of memory is relatively short. Autonomous vehicles, for example, can "read the road" and adapt to novel situations, even "learning" from past experience.
c) **Theory - of - mind AI** are fully - adaptive and have an extensive ability to learn and retain past experiences. These types of AI include advanced chat - bots that could pass the Turing Test, fooling a person into believing the AI was a human being. While advanced and impressive, these AI are not self - aware.
d) **Self - aware AI**, as the name suggests, become conscious and aware of their own existence. Still in the realm of science fiction, some experts believe that an AI will never become conscious or "alive".

2) Link between Artificial Intelligence and Nanoscience

The development of modern science and technology depends entirely on information, nano, and biological sciences. The thought of biology, artificial intelligence and nanotechnology convergence promoting a scientific and technical revolution has been lingering for more than a decade now. Although, this multidisciplinary research expected integration is still in progress. Knowledge of engineering, chemistry and physics is combined by nanotechnology meanwhile artificial intelligence highly depends on the biological inspiration for developing some of its most effective paradigms, for instance, evolutionary algorithms or neural networks.

If the link between current artificial intelligence and nanosciences is bridged then it is capable of boosting research in these disciplines and offering communication technologies and information to the new generation which will impact our society on a large scale, and possibly will provide the means for the merging of biology and technology. Alongside this, tools have been used by different efforts from artificial intelligence in basic and applied nanoscience research, for instance, for interpreting the experimental techniques or for helping in the structural design of devices and nanomaterials [24].

Unknown or complex data or functions can be represented and generalized by Machine learning methods, and when it comes to the treatment of interacting parameters, they are very efficient. The machine learning methods contain Methods like artificial neural networks (ANNs), an interconnected node - set in which an unsupervised or supervised algorithm determines the connection weights for learning input - output functions of these types. Search and optimization problems are being solved by other types of evolutionary or genetic algorithm - based bio - inspired AI paradigms [25]. Machine learning approaches are in a broad range, using combined or single methods containing;

decision trees, Bayesian networks, support vector machines (SVM) etc. And it can be implemented for complex classification, control problems, data mining, prediction, association, and clustering problems in the nanotechnology research context. In addition, nano computing, nanodevices, and nanomaterials provide increased power as effective architectures for implementing machine learning methods and AI, and generally, computer science can get an advantage from that increase in power. This bidirectional interaction between nanotechnology and AI has various usages and applications.

3) Artificial Intelligence's Application in Nanotechnology

Artificial intelligence has been an increasingly growing area for many decades now, not just within itself where the areas of Machin learning, Deep learning, and artificial neural network work simultaneously, but also in the number of fields and industries that they are now prevalent in. Nanoscience and nanotechnology are the study and application of tiny things. there are some growing areas where AI converges with nanotechnology [26].

During the last decade, there has been increasing use of artificial intelligence tools in nanotechnology research. In this paper, we review some of these efforts in the context of interpreting scanning probe microscopy, simulations, nanocomputing, food science, chemical modelling, Medical science and Nanobots.

a) AI in Scanning Probe Microscopy

Scanning probe microscopy (SPM) is the commonly used imaging technique in the nanoworld [27 - 28]. Numerous strategies that obtain images by the interaction between a pattern and a probe fall beneath this concept. Characterization of the pattern topography is accomplished by using the tunneling current between the pattern and the probe through their interaction. Several techniques have been developed by varying interactions among the tip and the sample, after the invention of nanoscope. SPM is likewise an effective tool for an atomic - scale manipulation. ANNs are extensively used for the categorization of various behavioral, structural, and physical properties of nanomaterials on the nanoscale, which are used in plenty of applications, viz., CNT (carbon nanotube), quantum - dot semiconductor optics and devices, chemical technology and production industry.

b) Nanoscale Simulation

One of the major issues which scientists have to face when working at the nanoscale is related to the tool simulation being studied [28] as actual optical pictures at the nanoscale cannot be achieved. Images must be interpreted at this scale, and numerical simulations are once in a while the best technique to get an accurate scheme of what is present in the image. Nonetheless, they are still tough to apply in many conditions, and lots of parameters need to be taken into account on the way to get a reasonable system depiction. Here, AI can be useful in enhancing the simulation's performance and making them simpler to collect and interpret. The use of ANNs in numerical simulations has been proven to be beneficial in various approaches when operating at the nanoscale. First, the software program can be manually modulated to control the stability between numerical exactness and physical implication. Another use of ANNs in simulation software is to lessen the complexity of configuration related to them (Castellano - Hernandez et al.2012).

c) Nanocomputing

There is a vast diversity of applications that emerge from the mixture of AI and current and upcoming nanocomputing methods [29 - 30]. Machine learning tactics implemented with the aid of nano - hardware to a certain extent to semiconductor - based hardware can also provide a foundation for a new technology of less costly and transportable era that can comprise high overall performance computing, including programs, sensory facts processing, and control tasks (Uusitalo et al.2011; Arlat et al.2012). The best expectations from the nanotechnology - enabled quantum computing and storage can considerably boost our capacity to clear up very complicated NP - whole optimization dilemma. Such sorts of issues arise in many unique contexts, but mainly those in big data that requires "computational intelligence" (Ladd et al.2010; Maurer et al.2012). In DNA computing, a lot of variables are in use [31]. This is a scenario in which DNA computing AI strategies are useful for purchasing an ultimate result from a minor preliminary data set, preventing the usage of all candidate solutions. Evolutionary and GAs are another options that may be considered.

d) Food Science

Food science is growing quickly in association with nanotechnology. The food market technology that is vital to hold marketplace leadership within the food processing industry in order to produce reliable, suitable, and tasteful fresh food products, and nanotechnology is the answer. Nanoparticles are used as preservatives and wrapping, respectively. Nanoscale food additives may be used to have an effect on product taste, nutrient composition, shelf life, and texture; may be used even to pick out pathogens; and may act as signs of meals' quality. Nanotechnology presents an enormous array of possibilities for the development of recent products and meals' system applications. AI strategies are pretty supportive for research and development possibilities for food additives and packaging.

f) Chemical modeling

A similar revolution has been quietly occurring in the world of chemical modeling. Chemical modeling simulates how molecules will interact with each other. It's used widely in bioscience and drug development. More recently, however, scientists have begun using the same modeling techniques to better understand the behavior of materials at the nanoscale and thereby have been able to improve their efficiency and efficacy. Neural networks have been used for chemical modeling for years, but it's only recently that they've been applied to nanotechnologies specifically towards understanding how nanotech materials behave under real - world conditions. AI is being used, for instance, to understand carbon nanotube structures by quantifying structural qualities like alignment and curvature. Using AIs, scientists and engineers can now minimise the degree of error related to the geometry or size of a system or particle. The most popular approach to doing this is to train an AI

model on data emerging from systems whose behaviour is already well understood.

g) Medical Science

Nanomedicine offers new ways for preventing and treating diseases [32]. However, reaching the full potential of nanomedicine is still yet to be fully realised. The use of automation is a step in the right direction of manufacturing nanoscale drugs. In order to improve and ensure that nanomedicine will achieve its desired result, computational analysis of large amounts of data must take place. Therefore, the next step is integrating AI and machine learning into the evaluation and formulation of nanoscale drugs. While traditional computational methods require deep understanding of the physical, chemical and biological knowledge to construct relevant and accurate computational models, AI algorithms require only training datasets that can be produced by automated synthesis practices, or sourced from the literature. Providing large datasets of experimental results related to the subject of study allows the algorithm to produce accurate prediction models that then can be translated into improved nano - formulations. There are multiple areas where machine learning can be integrated into nanomedicine applications. For example, machine learning can be used to improve the understanding of how the structure of a nanoparticle affects its characteristics as well as its interaction with targeting tissues and cells. Alternatively, the AI subfield can help determine the correlation between drug dosage and therapeutic outcomes. A recent study obtained gene expression profiles from 82 breast cancer patients and trained a machine learning algorithm to predict complete pathologic responses with an accuracy of 92% [33]. It should also be noted that there are algorithm approaches that can be used when there is not enough data available to train the algorithm.

h) Nanobots

Nanobots are robots that are microscopic in nature, measured largely on the scale of nanometers. They are currently in the research and development phase, but on realization, they are expected to do specific tasks at the atomic, molecular and cellular level and help in bringing about many breakthroughs, especially in medical science [34]. Nanobots are also known as nanomachines, nanorobots, nanomites, nanites or nanoids. The circulatory system of living beings is a natural highway for nanobots which will cruise through the bloodstream to the area of distress. They may be used to attach themselves to specific cells, such as cancer cells, and report the position and structure of these tissues. Nanobots can be considered to be a machine version of a bacteria or virus. They can be biological or synthetic but are adapted to perform preprogrammed tasks at the atomic level. They are expected to aid in research related to cancer, AIDS and other major diseases as well as in helping brain, heart and diabetes research. Other applications where nanobots can potentially be of use are in aerospace, security, defense, electronics and environmental protection [35].

4) Nano Science and AI in the future

There are bright and dark spots in the future of nanotechnology. On the one hand, the sector is expected to grow globally, driven by technological advances, increased government support, increased private investment and growing demand for smaller devices, to name a few. However, the environmental, health and safety risks of nanotechnology and concerns related to its commercialisation could hamper market expansion.

Artificial Intelligence has immensely benefited modern healthcare. Predictive analytics have helped foreseeing health issues, reduce medical cost, and market medicines. Disease diagnosis and decision making have been relatively simplified using image processing and machine learning. In addition, humanoid robots and precision machines have supported doctors during surgeries. Nanotechnology has influenced cancer research [36]and a major aspect has been developing effective and efficient drug delivery systems based on nanoparticles. Artificial Intelligence, and Micro - and Nano - electrochemical systems (MEMs and NEMS) [37] have worked in collaboration to assist doctors by developing algorithms and tracking the path of the transmitters attached to the nano - formulated drugs.

2. Conclusions

Artificial intelligence is a very key concept and methodology used in the field of computer sciences. It has been initiated for quite a time now but with that, the incorporation of nanotechnology has also been brought into this field, and ever since that it has proved to be extremely helpful and beneficial for the said field. A lot of work has been done and a lot of it is still in progress but it is true that it surely has brought an evolution in the field of science and technology. AI could efficiently offer solutions to many problems arising in the study of nanotechnology. It has been explored the use of ANNs and GAs in many exclusive contexts ranging from data interpretation in microscopy scanning probe to the characterization and category of nanoscale cloth properties. These pioneering efforts call for a real convergence of nanotechnology and AI in high - performance computer systems enabled by means of Convergence of AI and Nanotechnology primarily biomaterial - based nanocomputing devices. Of course, both AI and nanotechnology are emerging technologies, and it remains to be seen how each will develop. However, the ways in which these technologies are already being used mean that it's possible to see an emerging syncretism. Advances in AI are allowing us to understand the behavior of materials at the nano scale, and this is turn might allow us to create ever more powerful AIs. In this sense, the two technologies are closely intertwined.

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