JETIR.ORG ISSN: 2349-5162 | ESTD Year : 2014 | Monthly Issue
JOURNAL OF EMERGING TECHNOLOGIES AND INNOVATIVE RESEARCH (JETIR)
An International Scholarly Open Access, Peer-reviewed, Refereed Journal

ICT USES FOR GREEN, NANO, MEDICINE AND SYNTHETIC CHEMISTRY

Prof. Miss. Prachi Totaram Sarkate

U.G. Department of Chemistry, Late Baburao Patil Arts and Science College, Hingoli.

ABSTRACT –

IT plays an important role in education. ICT in education is an educational method which is used for information and communications technology to support, improve and optimize the dissemination of information. Studies investigating students' IT skills in chemistry in particular and science in general demonstrate that IT-enabled learning environments play an important role in education. While this may seem true in terms of overall assessment, the future is still influenced by innovations, which develop rapidly and in many ways are unpredictable. Computational chemistry is a branch of chemistry that uses computer excitement to help solve a chemical problem. It utilizes the theoretical chemistry methods which is integrated into computer programs to calculate the structure and their properties of molecules and different solids.

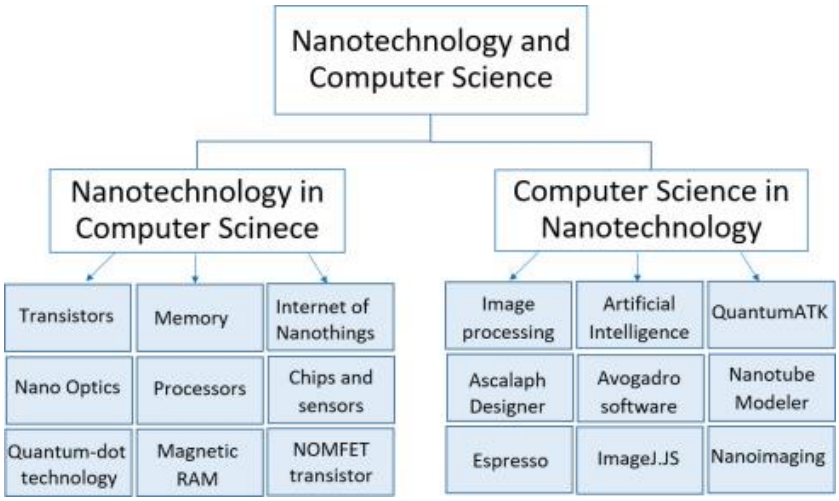
KEYWORDS –

ICT, Green, Nano, Medicinal and synthetic chemistry, Software.

INTRODUCTION –

ICT technology is used to develop new methods of analysis and synthesis to improve the accuracy and precision of measurement and automate the process. It examines and embodies visualizations in research facilities such as atomic demonstration, information collection, and introduction. We center moreover on ICT utilize by means of the World Wide Web (WWW) and virtual reality as well as the part of ICT for creating higher order considering abilities, such as request, graphing, docking and modelling. There are a few cases of distinctive assignments for educating chemistry utilizing ICT are presented counting a few suggestions for the planning of unused ones ICT tools play a significant role carrying out various chemical research activity such as Molecular Docking, database searching, chemical analysis, stimulation, molecular modelling. Various ICT tools are used in

teaching and research in chemistry. The uses of ICT in green, Nano, medicinal and synthetic chemistry are as follow-



1.GREEN CHEMISTRY –

The study and application of ecologically sustainable computing, often known as green IT (Information Technology), or ICT sustainability, is called green computing. Like green chemistry, green computing focuses on reducing the use of hazardous chemicals, enhancing energy efficiency over the course of the product's lifetime, and improving the recyclability and biodegradability of obsolete goods and industrial waste. Green computing is critical to all system kinds, from small handheld devices to massive data centers. To lessen the impact of their IT operations on the environment, many corporate IT departments have implemented green computing projects.[1]

2.NANO CHEMISTRY –

The potential to see, estimate, operate, and create resources at the nanoscale scale—which is equivalent to the size of molecules and atoms—is called nanotechnology. Numerous scientific and practical domains, such as computer technology, electronics, well-being, and farming, are affected by nanotechnology. In addition, computers are crucial for modeling and examining the characteristics of nanoparticles. Simulating and improving the process of developing nanotechnology is possible using computers thanks to their functionality [2],[3].Both the significance of nanotechnology for the development of computer technology and the purpose towards computer applications in nanotechnology were highlighted in earlier research investigations [4], [5].Two faces of the transferable link between computer science and nanotechnology are examined in this paper. The development of computer systems using nanotechnology is the first aspect. The role of computer systems applications is related to the simulation of nanoparticles behavior and studying their properties. The structure of transistors is the main factor in the ancient electronic memory schemes. The roles and relations are highlighted in the following sections. The important thing is the application of Nanotechnology is in computer systems also.

The part of computer science in nanotechnology is talked about in this segment with specific consideration paid to computer incitement the enhancement of Nano picture examination and the application of manufactured insights in nanotechnology. Since conducting inquire about at the nano scale is costly and in fact troublesome, researcher is prompted to utilize computational strategy to form the conduct of man structure.[6], [7], [8], [9]. Concurring to models utilizing tall k dielectric in capacitor will increase their capacitance to the specified level for ask for active random get to memory. The applications of Nanotechnology are specified within the taking after section-QuantumATK, Ascalaph Architect, Avogadro program, Nanotube modeler, Picture preparing methods in Nano images, Artificial insights (AI) in nanotechnology. SEM and TEM are mostly used for the nanoparticles in Nano chemistry.

3.MEDICINE CHEMISTRY –

ICT is used in Drug synthesis for their 3D structure their molecular analysis and in their studies. It also used to give the ability for enhancing the systems efficiency and preventing the errors of medical in health care [10]. Well-being statistics technology grant for new and more effective method to approach, communicate, activity, and store data Computers are mostly used in The field of medical profession. There are many steps of interface of medicine chemistry and computer technology. For the synthesize of drug and their characterization ICT helps a lot.

Data Analysis in Medicine-Large amounts of data are collected for medical study. It is important to compile, examine, and interpret this data. To achieve this, specific statistical techniques must be used, such as standard deviation and standard error calculations, as well as statistical significance tests like the Z test, paired and unpaired t tests, and chi-square test. Statistical techniques take a lot of time. Numerous statistical computations can be completed quickly with the aid of a computer[11].

Medical imaging-Computers have been widely employed in the past ten years to create high-resolution images. Such images can only be produced by specialized hardware and software in gamma, CT, MRI, and ultrasound cameras. This work is connected to the main hospital information system. It uses 3D representations of anatomy of humans, their physiology, and biochemistry in both health and illness.

4.SYNTHETIC CHEMISTRY –

In synthetic chemistry we synthesize compounds. And for the confirmation of this compound, we need NMR, IR, UV MASS and we get those results on computer through instrumentation. Then we do molecular docking process for the protein ligand binding site. For this docking we need different software like Auto dock vinna, Pymol, RasMol is used for the visualization of molecular structure and creating interactive stimulation of chemical process via, web browser through Rasmol. There is online computational tools for molecular modelling and for calculating chemical descriptor e.g., Chem axon, FAME, vortex etc. There is also some database sites like

chemicool, pubchem, chemspider, Cambridge structural database, SciFinder, The IUPAC gold book etc. Some ICT tools are used for Aromaticity, conversion of 2D to 3D, Tautimeric form,3D structure atomization, editing of molecular structure, auto renumbering etc. PubChem and Chem draw is the software from that we get the information about IUPAC name to structure and structure to IUPAC name.

REFERENCES–

1. Curry, B. Guyon, C. Sheridan, and B. Donnellan, "Developing a Sustainable IT Capability: Lessons From Intel's Journey," MIS Quarterly Executive, vol. 11, no. 2, pp. 61–74, 2012.
2. Babatunde D.E., *et al.*Environmental and societal impact of nanotechnology IEEE Access, 8 (2019), pp. 4640-4667
3. Merkle R.C.Computational nanotechnology Nanotechnology, 2 (3) (1991), p. 134
4. Karjala D.S.Protecting innovation in computer software, biotechnology, and nanotechnology Va. JL Tech., 16 (2011), p. 42
5. Jadhav S.S., Jadhav S.V.Application of nanotechnology in modern computers 2018 International Conference on Circuits and Systems in Digital Enterprise Technology, ICCSDET, IEEE (2018)
6. Kumar S., *et al.*Nanotechnology in computers Int. J. Inf. Comput. Technol. (2014), pp. 0974-2239
7. Rafiee R., Moghadam R.M.On the modeling of carbon nanotubes: A critical review Composites B, 56 (2014), pp. 435-449
8. Tian P.Molecular dynamics simulations of nanoparticles Annu. Rep. Sec. C(Physical Chemistry), 104 (2008), pp. 142-164
9. Guz I.A., Rushchitsky J.Computational simulation of harmonic wave propagation in fibrous micro-and Nano composites Compos. Sci. Technol., 67 (5) (2007), pp. 861-866
10. Winkler D.A.Recent advances, and unresolved issues, in the application of computational modelling to the prediction of the biological effects of nanomaterials Toxicol. Appl. Pharmacol., 299 (2016), pp. 96-100
11. Brown RA, Swanson BJ. Medical Statistics on Micro Computers. *Plymouth. Latimer Trend and Company Limited.* 1992:6–7