



Indian National Science Academy
New Delhi



Indian Academy of Science
Bangalore



The National Academy of Science
Prayagraj

SCIENCE ACADEMIES' VIRTUAL LECTURE WORKSHOP ON


EMERGING TRENDS OF COMPUTATIONAL METHODS IN DRUG DEVELOPMENT

6-7 November, 2020

Organized by
Department of Physics, NERIST



REGISTRATION LINK:

<https://docs.google.com/forms/d/e/1FAIpQLScIsF6ZAphYNR4qGgvtd9nzkgvq67BOEIXkH3cSML-pJgA2eg/viewform> 

- Registration is mandatory and free.
- Workshop link will be sent via email to registered participants.
- The workshop is opened to PG students and faculties of technical and non-technical Colleges and Universities.
- E-certificate of the participation will be issued to the participants after the completion of the Lecture workshop.

Objective: Molecular modelling plays a vital role in finding out new drugs needed for the treatment of dreadful diseases. Computational methods are used in computational chemistry, drug design, material science and computational biology to elucidate the structural and dynamical behaviour of the molecules. It is imperative to bring awareness of its usefulness to the larger audience, especially during this COVID -19 pandemic.

Resource Persons

Prof. Biman Bagchi, FNA, FNASc, FASc, FTWAS,
Honorary Professor, SSS Chemistry unit, IISc Bangalore

Prof. Sandip Paul, Professor, Department of
Chemistry, IIT Guwahati

Prof. Sanjay Kumar, FASc, Professor, Department
of Physics, BHU, Varanasi

Dr. Hubert Joe, Associate Professor, Department of
Physics, MIC, University of Kerala

Convener:

Prof. Yashwant Singh, F.A.Sc, F.N.A, F.N.A.Sc
Distinguished Professor
Department of Physics
Banaras Hindu University, Varanasi

Coordinator:

Dr.Th. Gomti Devi
Associate Professor
Department of Physics
North-Eastern Regional Institute of Science and
Technology, Arunachal Pradesh
Email: inavlw2020@gmail.com, Ph-9436229323

About the Lecture workshop:

Molecular modelling plays a vital role in finding out new drugs needed for the treatment of dreadful diseases. It includes all theoretical and computational methods to mimic the behaviour of molecules such as small chemical molecules, drugs, proteins and enzymes, respectively. Molecular modelling includes molecular dynamics, quantum mechanical methods, molecular mechanics methods, molecular dockings and conformational analysis, respectively. This Virtual lecture workshop brings awareness of the importance of computational methods in finding out potential drugs of the dreadful diseases to larger audience, especially during this COVID -19 pandemic. The role of the molecular modelling in finding out new drugs and the different methods of computation used in solving the drug-ligand/drug-receptor interaction is to discuss in this platform. The 2-Day virtual lecture workshop organized by Department of Physics, NERIST with the Joint Science Education Panel of the three Science Academies - Indian National Science Academy (INSA), New Delhi, Indian Academy of Sciences (IASc), Bengaluru and The National Academy of Sciences India (NASI), Prayagraj shall be beneficial to the students, young researchers and teachers across the region to explore the potential of computational methods in designing and development of drugs. The Lecture workshop is incorporated with the invited lectures in basic, current and frontier areas of theoretical modelling by eminent academicians/ scientists.

Topics to be covered

Basic idea of molecular modelling, types and applications

Soft matter and applications

Modelling of biopolymers

Molecular modelling in drug development

Different computational methods in drug development

IMPORTANT DATES

The last date for the receipt of applications:

30th October 2020

Intimation of selection by email:

2nd November 2020

About the Institute:

The North-Eastern Regional Institute of Science & Technology(NERIST) is a unique Institute of its own kind in the country, having unconventional and innovative academic programmes. It is an autonomous Institute under MOE, Government of India. It was established in 1984 to produce technical manpower at various levels and to meet the technical requirements for all round development of the North-Eastern States. NERIST got the status of deemed to be university on 31st May 2005 under section 3 of the UGC Act 1956. It offers modular pattern of education in all the disciplines of Engineering along with Forestry as an applied Science discipline. It also offers various Postgraduate Courses viz, M.Sc., M.Tech., M.B.A and Doctoral Programmes in all branches of Engineering, Applied Science, Physics, Chemistry, Mathematics, Management and Humanities.

About the Department:

The Department was established along with the Institution in the year 1986. The Department of Physics offers eight core courses for the undergraduate students at different levels (Base, Diploma, and Degree modules) of Engineering and Applied Science Streams. Apart from this, the department has been offering M.Sc. course for the Postgraduate students since 2009. The Department of Physics is a DST-FIST sponsored department having sophisticated high-end research instruments such as, X-ray diffractometer, Laser Raman Spectrometer, broad frequency Impedance Analyzer and Differential Scanning Calorimeter in FIST lab. The faculty members are actively involved in research activities and have been publishing research papers in both national and international journals.

Speakers:

1. Prof.Biman Bagchi, FNA, FNASc, FASc, FTWAS,
Honorary Professor, SSS Chemistry unit, IISc Bangalore
2. Prof. Yashwant Singh, FNA, FNASc, FASc,
Distinguish Professor, Department of Physics, BHU
3. Prof. Sanjay Kumar, FASc, Professor, Department of Physics, BHU
4. Prof. Sandip Paul, Professor, Department of Chemistry, IIT Guwahati
5. Dr. Hubert Joe, Associate Professor, MIC, Department of Physics, University of Kerala
6. Dr.Th.Gomti Devi, Associate Professor, Department of Physics, NERIST