



National Workshop on Hands on Training Using In-Silico Tools for Chemical / Biological Applications

14th - 16th October 2023 (Saturday to Monday) **OFFLINE**

17th October 2023 (Tuesday) **ONLINE**

SPEAKER



Dr. K. Bhanuprakash

Chief Scientist (Retd.),
IICT Hyderabad.

Title of the talk:

Computational Chemistry to
Predict and Understand
Molecular Properties



SPEAKER

Dr. D. L. V. K. Prasad

Professor, IIT Kanpur

Title of the talk:

Atoms, Molecules and
Photons: Simulations and
Uncertainties



VIGNAN'S

Foundation for Science, Technology & Research

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-Estd. u/s 3 of UGC Act 1956



Organised by: Department of Chemistry
School of Applied Science & Humanities



About our University

Vignan's Foundation for Science, Technology & Research is an institute, which provides quality education in a diverse and intellectually stimulating environment. It imparts value addition training to students to make them competent and inspired engineers.

The Institute celebrates the power of knowledge, cultivates vision and encourages new ideas, besides aiming to inculcate human values and build awareness about the self and society around. The Institute is well known for its dedicated faculty, state-of-the-art infrastructure and excellent Placement Record.

As a University, it is in the process of improving its standards to the level of a global technical institution. The latest curriculum has been prepared after consulting the institute's illustrious alumni working across the world, veterans from industry and distinguished academics possessing a rich teaching and research background. Living up to its motto, 'Technology with a Human Face', the institution imparts knowledge and skills, while instilling human values and awareness about self and society. In the recent nationwide survey of Indian universities carried out by NIRF, VFSTRU was placed at 75th rank. The University is ISO certified and has been accredited by NBA and NAAC 'A+' Grade.

Department of Chemistry

The Department of Chemistry, working under the School of Applied Science and Humanities, has been catering to the needs of core engineering departments since 1998 and offers various courses like, Engineering Chemistry and Organic Chemistry theory and lab courses for B. Tech. students. The Department of Chemistry has offered M.Sc. Chemistry and M.Sc. Organic Chemistry since 2020. The Chemistry Department is served by a team of highly motivated, 20 Ph.D. faculty members from world-class institutes like Cornell University, the IITs, and Central University. It is also offering a Ph.D. program in all research specializations in chemistry. Under the Chemistry Department, 30 Ph.D. degrees have been awarded so far, and 90 more students are currently pursuing their Ph.D. program. Moreover, the Chemistry Department is also planning to offer B.Sc. (honors) and M.Sc. Analytical Chemistry from the coming academic year onward.

About the National Workshop

Importance of in-silico tools for various chemical and biological applications. Visualisation tools like Gaussview, pymol, discovery studio will also be taught in the session. Apart, the support will be given to the participants if they facing any problem during the calculations.

Name of the Trainers

Trainers	Tools will be taught	Teaching Assistant
Dr. V. Srinivasadesikan	Gaussian 16 suite of program	Mr. Anjanayulu
Dr. Sudip Mandal		
Dr. Viswajit	Autodock	Mr. Vidyasagar
		Mr. Sk. Sharif
Mr. Sharma	RESCUE	Mr. Naga Ashok

Schedule of the Workshop

Day 1 / Session 1	Date	Time	Speakers	Coordinator
Inauguration	14 th October 2023	9.30 to 10 AM	Conveners, Senior Professors, HoD, Dean, Registrar, Vice-Chancellor and Chairman	Mr. Nagaraju Mr. Perumal
Talk - 1		10.05 to 11 AM	Dr. Bhanu Prakash, IICT, Hyderabad	Mr. Anjanayulu
Tea Break				
Talk - 2	14 th October 2023	11.25 to 12.20 PM	Dr. DLVK Prasad, IIT, Kanpur	Mr. Perumal
Technical Discussion (Q & A)		12.25 PM to 1.00 PM	Dr. Bhanu Prakash, IICT, Hyderabad & Dr. DLVK Prasad, IIT, Kanpur	Mr. Naga Ashok
PHOTO SESSION				

Schedule of the Workshop

Date & Time	Trainers	Teaching Assistant	Tools will be taught	Applications
14 th October, 2023 02 to 05 PM	Dr. V. Srinivasadesikan Dr. Sudip Mandal	Mr. Anjanayulu	Gaussian 16 suite of program	Draw the Molecule using Gauss View SMILES - Introduction
15 th October 2023 09.30 AM to 05 PM	Dr. V. Srinivasadesikan Dr. Sudip Mandal	Mr. Anjanayulu	Gaussian 16 suite of program	<ul style="list-style-type: none"> • Introduction to HPC • DFT Methods and Basis sets • Optimization • Frequency Calculation • Frontier Molecular Orbital • Electrostatic Potential • Natural Bond Orbital (NBO) • Transition State Calculations • Spectroscopy like NMR, IR and UV • Solvent Phase (PCM & CPCM) calculations
16 th October, 2023 to 04.30 PM	Dr. Viswajit Department of Biotechnology, VFSTR	Mr. Vidyasagar Mr. Sk. Sharif	Autodock	<ul style="list-style-type: none"> • Introduction to Database • Search using protein ID • Autodock • Parameters setup • Molecular Docking • Result Analysis and Report Writing
REFLECTIONS & VALEDICTORY				
17 th October, 2023 06 PM to 08 PM (Online)	Mr. Deepak Upadhyay, Impulse Technology	Mr. Naga Ashok	RESCUE Software Package for Material Science Applications	Demo on RESCUE Software Package

Chief Patrons

Dr. L. Rathaiah
Chairman &
Chancellor, VFSTR

Sri L. Srikrishnadevarayalu
Vice-Chairman, VFSTR

Patrons

Dr. P. Nagabhushan
Vice-Chancellor, VFSTR

Ex. Comd.
Dr. M. S. Raghunathan
Registrar, VFSTR

Co-Patrons

Dr. G. Srinivasa Rao
Professor & Dean R&D, VFSTR

Dr. N. Srinivasu
Professor & Dean SASH

Dr. K. Prabhakara Rao
Professor & HoD Chemistry,
SASH

Organizing Committee

Dr. D. Nagaraju, Prof., Chemistry, SASH

Dr. N. Satya Sree, Prof., Chemistry, SASH

Dr. Sk. Anwar, Assoc. Prof., Chemistry & Assoc. Dean SASH

Dr. Anandarup Goswami, Assoc. Prof., Chemistry,
SASH & Assoc. Dean PCFA

Dr. M. Sireesha, Assoc. Prof., Chemistry, SASH

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Dr. Chandrasekar Kuppan, Assoc. Prof., Chemistry, SASH

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Dr. N. Satyavijaya Kumar, Asst. Prof., Chemistry, SASH

Dr. Shubhalakshmi Sengupta, Asst. Prof., Chemistry, SASH

Mr. K. Mariadas, Asst. Prof., Chemistry, SASH

Conveners:

Dr. V. Srinivasadesikan
Assoc. Prof., Chemistry,
SASH & Assoc. Dean IQAC

Dr. Sudip Mandal
Asst. Prof., Chemistry, SASH

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Registration Link :

<https://forms.gle/HLFJAsLzZwfjcw8s9>

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