



**DST-SERB Sponsored High-End
Workshop (KARYASHALA)**

on

Computational Chemistry and Molecular Design

April 12-18, 2024

Organized by

Department of Chemistry

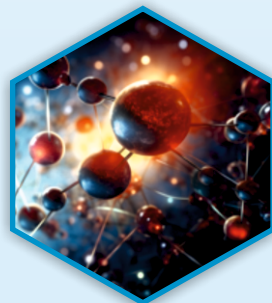
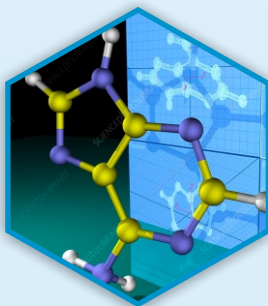
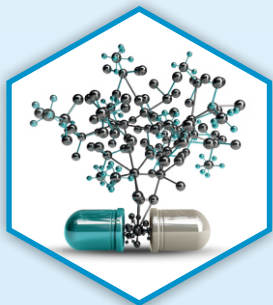
**Prof. Rajendra Singh (Rajju Bhaiya) Institute of Physical Sciences for Study and Research
Veer Bahadur Singh Purvanchal University, Jaunpur-222003, U.P., India**

Funded by :

Science & Engineering Research Board (SERB)

Department of Science & Technology (DST)

under the Accelerate Vigyan Scheme



About the University

Veer Bahadur Singh Purvanchal University (VBSPU) is a state university located in Jaunpur, Uttar Pradesh, India. It was established in 1987 and is named after Veer Bahadur Singh, the former Chief Minister of Uttar Pradesh. The university is recently accredited with A+ by NAAC.

The university aims to provide quality education and research opportunities to students. The university offers a wide range of undergraduate, postgraduate and doctoral programs in various disciplines including science, arts, commerce, pharmacy, law, management, engineering, technology, and computer applications.

The campus of VBSPU is spread over a large area with modern infrastructure facilities including libraries, laboratories, computer centers, sports facilities, and hostels for students. The university also promotes extracurricular activities and encourages students to participate in various cultural, sports, and social events.

About the Institute

Prof. Rajendra Singh (Rajju Bhaiya) Institute of Physical Sciences for Study and Research within the campus of Veer Bahadur Singh Purvanchal University, Jaunpur is an Institution of national reputation and established by the efforts of the Government of Uttar Pradesh, in the year 2018. The establishment of the Institute accomplishes the mission of the University to offer best environment for education, students and society for universal developments in all respects. The Institute has four departments of Physical Sciences viz: Physics, Chemistry, Mathematics and Earth & Planetary Sciences which offers the undergraduate, postgraduate and doctoral programme. Institute has two research centers i.e., Nanoscience and Technology Research Centre and Renewable Energy Research Centre which offer M. Tech. (Materials Science & Technology) programme. The departments and research centres have well-equipped laboratories with instruments like SEM-EDS, XRD, FTIR, UV Vis, APS-100, TPS-500S with other infrastructural facilities for undertaking advanced level research.

About the Department

The Department of Chemistry is one of the prominent departments of Prof. Rajendra Singh (Rajju Bhaiya) Institute of Physical Sciences for Study and Research in VBS Purvanchal University, Jaunpur campus. The Department offers M.Sc. and Ph.D. programme in Chemistry. Doctoral and post-doctoral researches are carried out in all major areas of chemical and allied sciences.

Faculty members in Chemistry department are well recognized and their areas of research are cutting edge and mainly focused on society current need and problems. The department is working to reshape the state's public higher education by training new generation postgraduate students engaging in interdisciplinary research, signing MoUs with industry and entrepreneurs that gave jobs opportunities to postgraduate students.

Department have access to the excellent facilities and sophisticated instruments in other departments and centres of the Institute. The Department offers a vibrant atmosphere to students to nurture the spirit of scientific temperament and to pursue pioneering research in a highly encouraging environment. Besides committed to excellence in teaching to postgraduate student, the faculty members and research scholars of the chemistry department are actively engaged in research to the different area of chemistry viz. computational chemistry, inorganic synthesis, coordination chemistry, organometallic in catalysis, perovskite solar cell.

About the Workshop

Computational chemistry has impacted how we see the world, helped manufacturers create more effective manufacturing methods, characterized new chemicals and materials, and assisted other researchers in mining massive amounts of data for relevant information. In essence, it has given qualitative and quantitative insights into experimental activity, directed the selection of the experimental system to be studied or allowed the construction of new systems.

The workshop aims to cultivate basics of computational chemistry in participants. Participants of this Workshop will learn how to use open source molecular editors & visualizers for building molecules (organic as well as inorganic) and materials (crystal structures, polymers, CNTs, quantum dots etc.). The workshop aims to cover followings topic in lecture and hands-on training

- Introduction to computational Chemistry
- Molecule builder and visualization tools.
- Basis sets and choice of theoretical methods
- Basics of Quantum Mechanical Calculations
- Introduction to Molecular dynamics
- Molecular Modelling
- Molecular Simulation



Eligibility : Students currently pursuing Masters or Ph.D. in Chemistry/Physics/ Material Science or relevant disciplines are eligible to apply. The number of participants for the workshop will be limited to 25. The selection of the candidates will be made by the screening committee as per SERB guidelines. Selected candidates will be intimated through email on 1st March, 2024. Participants are advised to bring their own laptop for the Hands-on sessions. The workshop will be conducted in physical mode.

Travel and Accommodation : Selected candidates will be reimbursed travel expenditure (Train fare up to sleeper class or state transport buses by the shortest route as per GOI norms). Food and accommodation will be provided by the organizers.

Application Procedure : To apply for the workshop, applicant must fill out the attached application form and get it approved from their guide/HOD/Competent authority. The selected applicant must bring the filled application form.

Registration : Applicant get registered **FREE** through following link -

<https://forms.gle/uBAyWrGBemBjdUew7>

Important Dates

Last Date of Registration
March 30, 2024

Intimation of shortlisted candidates
March 31, 2024

Commencement of Workshop
April 12, 2024

Organizing Committee

Chief Patron

Prof. Vandana Singh

Vice Chancellor

VBS Purvanchal University, Jaunpur

Patron

Prof. Pramod Kumar Yadawa

Director - Rajju Bhaiya Institute

Convener & Event Organizer

Dr. Nitesh Jaiswal

Course Coordinator

Dr. Ajeet Singh

Chairman

Dr. Pramod Kumar

Head, Department of Chemistry

Organising Secretary

Dr. Mithilesh Yadav
Dr. Dinesh K. Verma



ACCELERATE
राष्ट्रियज्ञान



Application (To be Uploaded Online)

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Department of Chemistry

Prof. Rajendra Singh (Rajju Bhaiya) Institute of Physical Sciences for Study and Research
Veer Bahadur Singh Purvanchal University, Jaunpur-222003, U.P., India

1. Name of Applicant :
2. Enrollment/Registration Number :
3. Degree (PG/PhD) :
4. Year of study (1st/2nd/Final) :
5. Department :
6. Institute/University :
7. Correspondence Address :
8. Mobile Number and e-mail ID :
9. Academic Record :

Affix Recent
Passport Size
Photo

Sl. No.	Examination Passed (up to current degree)	Subject (Major)	Year of Passing	Marks (%)/ CGPS
1.	Bachelor Degree			
2.	Master Degree			
3.	Ph.D.			
4.	Any other qualifications			

The above information provided is true to the best of my knowledge. If selected, I agree to abide by the rules and regulations of the program.

Date:

Signature of the application

Recommendation by the forwarding authority (Guide/HOD/competent authority)

Dr./Mr./Miss is hereby nominated for participating in the SERB sponsored High-end workshop at Department of Chemistry, Prof. Rajendra Singh (Rajju Bhaiya) Institute of Physical Sciences for Study and Research, VBS Purvanchal University, Jaunpu U.P. from 12-18 April, 2024.

Date:

Signature & Seal