

# RESEARCH SCOPE

ISSUE-1 (April, 2022)

## An Online Workshop on D.F.T. Investigation of the Electronic Structure using Quantum Espresso and BURAI Software (Atoms, Molecules, Compounds and Crystalline Materials)

An Online 9 Days workshop on D.F.T. Investigation of the Electronic Structure using Quantum Espresso and BURAI Software was organized by The Centre for Research, Innovation and Training (CRIT), IIS (Deemed to be University), Jaipur in collaboration with Gramin Mahila Mahavidyalaya, Sikar (Rajasthan), from 9 to 17 February, 2022. It was attended by 145 participants.

In the 26 technical sessions the participants were enlightened about various scientific topics & areas like, Introduction to Quantum Espresso, Structure of Input Files & Installation of BURAI, Fermi Surfaces, D.F.T. : Introduction and Applications, Electronic Structure of Atoms & Molecules, Revisiting the Landscape of Theoretical Modeling using DFT, Checkpoints of DFT Calculation, Electronic Structure of GaAs using BURAI, Effective Carbon dioxide Utilization Methods: Challenges and Opportunities, Applications of Quantum Espresso in Advanced Multi-functional Materials, use of WIEN2K software for bandgap calculation, Measurement of Energy Diagram of an Oscillator using 'Tracker' Software & Calculation of Reactivity Descriptors using Gaussian Software.

Hands-on training was also given during numerous sessions on calculations of Electronic Structure of Atoms (like H & N) and molecules (like CO<sub>2</sub>, NH<sub>3</sub>, H<sub>2</sub>O) 2D Material (GeS<sub>2</sub>), Compounds (like HCl, NaCl), Topological Insulators (like Bi<sub>2</sub>Te<sub>3</sub> & Sb<sub>2</sub>Te<sub>3</sub>) by using BURAI, Construction of Super Cell & Impurity Doping; Modeling for Surface Studies by taking example of copper crystal & Electronic Structure of BaTiO<sub>3</sub> Perovskite were also discussed by using BURAI software.

### ONLINE WORKSHOP ON DFT INVESTIGATION OF THE ELECTRONIC STRUCTURE USING QUANTUM ESPRESSO AND BURAI SOFTWARE

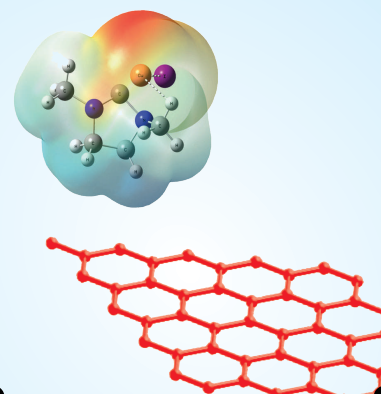
Atoms, Molecules, Compounds and Crystalline Materials  
09 - 17 FEBRUARY, 2022

Jointly Organised by

 Centre for Research, Innovation and Training (CRIT)  
IIS (Deemed to be University), Jaipur  
and  
Gramin Mahila Mahavidyalaya, Sikar, Rajasthan

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FROM THE  
DESK OF

Chancellor



**Dr. Ashok Gupta**

IIS (Deemed to be University), where Unique is a tradition, has been a vibrant cosmopolitan University since a quadri centennial in the Pink City, India. Accredited by NAAC and included u/s 12 B by UGC, IIS University has been a trailblazer since its inception in 1995 as the International College for Girls. Besides offering a wide array of semester based UG, PG and Research Programmes in numerous disciplines, it takes initiatives in implementing the innovative pattern of Teaching and Research as per the UGC regulations. The University is also approved by DSIR-DST as a Centre of Research and Development.

FROM THE  
DESK OF

Vice-Chancellor



**Prof. T.N. Mathur**

As Albert S. Gyorgyi says, "Research is to see what everyone else has seen and to think what nobody else has thought", IIS (Deemed to be University) ensures that the faculty and students are motivated to indulge in research and widen the circumference of their knowledge. It has its own Academic Research Bodies, like the Research Promotion Committee (RPC), CRIT and IQAC, to promote research-based activities amongst its faculty and students by facilitating research labs, funds, books, digital resources and research-friendly environment as required.

FROM THE  
DESK OF

Registrar



**Dr. Raakhi Gupta**

To ensure that everyone is driven by the spirit of inquiry in their quest for knowledge, IIS (Deemed to be University) brings out RESEARCHSCOPE, a quarterly magazine that encapsulates the research endeavours of the faculty and students, the awards bagged by them at various research-oriented activities and similar other attempts or events that aim at promoting and sharing research. The IIS family believes in what Father Keller says, "A candle loses nothing by lighting another candle" and therefore in lieu of the University's efforts towards the betterment of the global community, IIS invites people to take the torch of research forward through this compendium.

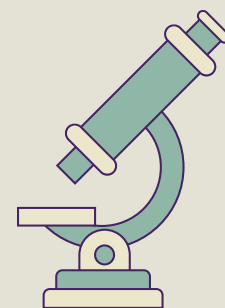
FROM THE  
DESK OF

Director CRIT



**Prof. K.S. Sharma**

IIS (Deemed to be University) has established RPC and CRIT (Centre for Research, Innovation and Training) that aim at enhancing research aptitude and building quality research capacity in its faculty and students through workshops, seminars, guest lectures, trainings and conferences revolving around research. These bodies promote academic integrity amongst the scholars, establish the culture required for ethical studies and upgrade strategies for quality enhancement of research. RESEARCHSCOPE is another endeavour of RPC and CRIT at IISU to foster research acumen in its members and share it with the society for global needs.



## DEPARTMENT OF PHYSICAL & COMPUTING SCIENCES

Discipline of Physics at IIS (deemed to be University) is among the departments which were established in the early stage of the university, in July 1995 and has since then grown into one of the major centres for teaching, learning and research at the IIS (deemed to be University).

### INNOVATIONS IN CURRICULUM

- ▶ Introduction of communications skills, Bio Physics, Medical Physics and Astrophysics in the syllabus of PG students.
- ▶ Papers on Contemporary topics like Renewable Energy, Nanotechnology have been incorporated in the syllabus of B.Sc. (H) Physics.
- ▶ Software like MATHEMATICA, MATLAB, WIEN 2K, Quantum Espresso, SPSS, P-Spice, R, Python, Scilab introduced in Practical courses at UG /PG level.
- ▶ Planning to start an Integrated Dual Degree Programme on B.Sc-M.Sc Nanoscience and Technology from the session 2022-23.

### RESEARCH INITIATIVES

- ▶ A sophisticated Thermal Vacuum coating Unit of HHV make (SMART COAT 3.0) in Thin Film and Nanotechnology Lab.
- ▶ Five Microwave benches of different frequencies are available in Microwave Research Lab
- ▶ For theoretical research, the cluster computing is proposed to be installed.

### FACULTY ACHIEVEMENTS



**Ms. Neeraj Kulhari** has been awarded a Scholarship under HPC Europa 3 Project to do research for 3 months (10 Jan.'22 to 3 Apr.'22) at

CNR-SPIN under the supervision of Dr. Alessandro Stroppa (Research Director at CNR-SPIN in Unit L'Aquila), Italy on study entitled "MOKE properties of AB stacking in  $\text{FeBr}_2/\text{FeCl}_2$  Heterostructures and BA stacking in  $\text{VBr}_2/\text{VCl}_2$  by using the Density Functional Theory".

### CONFERENCES AND ACTIVITIES

- ▶ Two days workshop on Experimental Techniques on Nano Sciences was organized for Faculty and PG Students of the Dept. of Physics on 18-19 April 2022.
- ▶ One day Interaction/ Technical talk with Prof. Chetan Singh Solanki, IIT, Bombay on "Energy Swaraj : Essence of sustainability" on 24th February, 2021.
- ▶ National Conference on Recent Trends in Material Science and Nanotechnology on 18-19, January 2019.

### BEST PRACTICES

- ▶ National Graduate Physics Examination (NGPE) by Indian Association of Physics Teachers (IAPT) is conducted every year.
- ▶ Department has an association with Prof Volker Heine, a leading scientist in the field of pseudo potential theory of metals and group theory. A Gold medal by the name "Prof. Volker Heine FRS Gold Medal for excellence in Physics at IIS(deemed to be University)" has been instituted from the session 2020 -21 by Prof. Volker Heine FRS, Cavendish Laboratory (TCM), J J Thompson Ave. Cambridge, England .
- ▶ Workshops, symposium and training sessions are arranged to enable students to learn and interact with scientists and researchers from all around the country on different specialised topics in physics.

### INSTITUTIONAL MEMBERSHIP FOR ENERGY SWARAJ FOUNDATION





## BEST PUBLICATIONS DURING LAST 5 YEARS

- Soni, G., Gouttam, N., Joshi, V. (2022). Synthesis and comparisons of Optical and Gamma Radiation shielding properties for ZnO and SiO<sub>2</sub> nanoparticles in PMMA nanocomposites thin films. *Optik*, 259, 168884 (IF 2.443).
- Faizan, M., Bhamu, K. C., Murtaza, G., He, X., Kulhari, N., Al-Anazy, M. M., & Khan, S. H. (2021). Electronic and optical properties of vacancy ordered double perovskites A<sub>2</sub>BX<sub>6</sub> (A = Rb, Cs; B = Sn, Pd, Pt; and X=Cl, Br, I): a first principles study. *Scientific reports*, 11(1), 6965. (IF 4.379).
- Soni, G., Jangir, R.K. (2021). Effect of temperature on nano graphite doped polymethylmethacrylate (PMMA) composite flexible thin films prepared by solution casting: Synthesis, optical and electrical properties. *Optik*, 226(1), 165915. (IF 2.443).
- Soni, G., Srivastava, S., Soni, P., Kalotra, P., Vijay, Y. K. (2018) Optical, mechanical and structural properties of PMMA/SiO<sub>2</sub> nanocomposite thin films. *Materials Research Express*, 5, 015302 (IF 1.61).
- Sharma, R., Khan, S., Goyal, V., Sharma, V., Sharma, K. S. (2017). Investigation on effect of boron and nitrogen substitution on electronic structure of grapheme. *FlatChem*, 1, 20-33. (IF 5.227).

**21 PUBLICATION BY THE DISCIPLINE DURING LAST 5 YEARS**

**408 TOTAL NUMBER OF PUBLICATIONS BY THE FACULTY**

**06 NUMBER OF UNIVERSITY RECOGNIZED RESEARCH SUPERVISORS**

**03 Ph.D. DEGREE AWARDED**

**09 NUMBER OF CANDIDATES ENROLLED FOR Ph.D.**

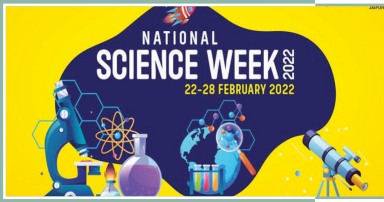
## THRUST AREAS

- Measurement of dielectric properties of solids and liquids at microwave frequencies.
- Electronic Structure studies of materials using WIEN2K and Quantum Espresso.
- Deposition of thin films of different materials using vacuum coating thermal evaporation system (Hind high Vacuum: Smart 3.0A) and study of their properties.
- Synthesis of nanoparticles using sol – gel method and hydrothermal method.
- Renewable Energy Technology.
- Designing and study of Electronic Circuits.





# RESEARCH BASED ACTIVITIES



National Science Week on the theme **Integrated Approach in Science and Technology for Sustainable Future**, celebrated in the University, organized by Faculty of Science from 22-28 February 2022



2 days 2<sup>nd</sup> FICR International Conference on **Rising Threats in Expert Applications & Solutions**, organized by Department of Computer Science and Information Technology, on 7-8 January 2022 in hybrid mode



National Workshop On **Data Analysis Through SPSS**, organized by department of Economics from 20-24 December 2021



Online Workshop on **How to Catch Cloned/Fake/ Predatory Journals in Academics**, organized by Centre for Research Innovation and Training, IIS (deemed to be University) Jaipur on 10 November, 2021

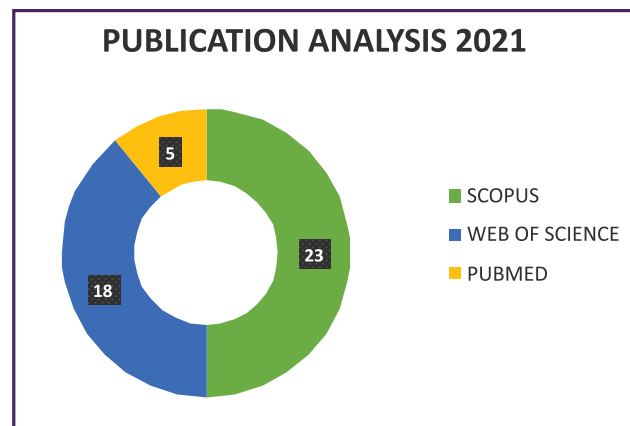
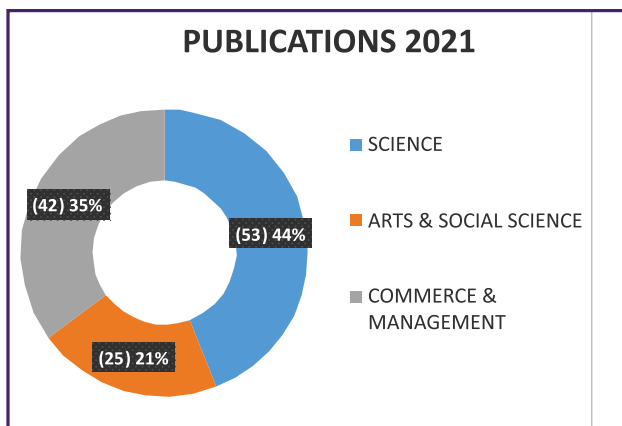


Three day 8<sup>th</sup> Rajasthan Science Congress on **Science and Technology for Sustainable Development**, organized by IIS deemed to be University, Jaipur, from 20-22 October 2021



Online Workshop on **Identifying Reputed Journals for Publication**, organized by Centre for Research Innovation and Training (CRIT) on 18 September, 2021

# PUBLICATION STATUS



# FACULTY AWARDS

<b>Dr. RICHA BHARADWAJ</b>	Best oral presentation at International Conference on Advances in Biotechnology and Applied Microbiology organized by IIMT University Meerut, 30-31 March, 2022.
<b>Ms. REENA VERMA</b>	Platinum award and a cash prize of Rs. 25000/- for best research paper in All India Inter University Research and Innovation Festival organized by Ravindra Nath Tagore University, Bhopal, 25-26 March, 2022.
<b>Dr. ANJU SHARMA</b>	Best oral presentation at International Conference on Multidisciplinary Approaches to Environmental Research for Human Health, organized by University of Rajasthan, Jaipur, 24 December, 2021
<b>Dr. NEELU KANWAR RAJAWAT</b>	Young Researcher Award at National Conference on Environmental Toxicology, organized by Vivekananda Global University, Jaipur, 25-26 November, 2021 .
<b>Ms. VYOMA AGARWAL</b>	Best Poster presentation at 4th International conference on Food and Nutrition, Singapore, organized by Universal Society of Food and Nutrition, 23-24 September 2021

## Ph.D. AWARDED (July 2021-April 2022)

### Arts & Social Sciences

- ▶ Ms. Surbhi Jain (English)
- ▶ Ms. Afifa Baig (Journalism)
- ▶ Ms. Reeva Chaudhary (Psychology)
- ▶ Ms. Jolly Jain (Journalism)
- ▶ Ms. Ruchi Sharma (English)
- ▶ Ms. Vrinda Chauhan (Sociology)
- ▶ Ms. Nandini Agarwal (Economics)
- ▶ Ms. Ankita Choudhary (English)
- ▶ Ms. Kritika Agarwal (Fine Arts)

### FUNDING AGENCIES for Extra Mural Projects

- ▶ UGC - <https://www.ugc.ac.in/>
- ▶ ICSSR - <https://icssr.org/research-projectsmajor-and-minor>
- ▶ AYUSH - <https://main.ayush.gov.in/>
- ▶ DST - <https://dst.gov.in/>
- ▶ DBT - <https://dbtindia.gov.in/>
- ▶ MNRE - <https://mnre.gov.in>
- ▶ CSIR - <https://www.csir.res.in/>

### Commerce & Management

- ▶ Ms. Ruby Singh (Management)
- ▶ Ms. Amita Sharma (Management)
- ▶ Ms. Khushbu Bhardwaj (Management)
- ▶ Ms. Pratishtha Bhardwaj (Management)
- ▶ Ms. Ankita Rathore (Management)
- ▶ Ms. Swati Chaudhary (Commerce)
- ▶ Ms. Ankita (Commerce)
- ▶ Ms. Aanchal Kalra (Commerce)
- ▶ Ms. Natasha Swami (Commerce)
- ▶ Ms. Sakshi Joshi (Commerce)
- ▶ Ms. Kiran Khinchi (Commerce)
- ▶ Ms. Neha Adlakha (Management)
- ▶ Ms. Yogita Khatri (Management)
- ▶ Ms. Ati Jain (Commerce)
- ▶ Ms. Akanksha Kumari (Commerce)
- ▶ Ms. Neha Sukheja (Commerce)
- ▶ Ms. Juhi Mukharjee (Commerce)
- ▶ Ms. Adra R. Nair (Commerce)
- ▶ Ms. Himani Sharma (Management)
- ▶ Ms. Honey Goyal (Management)
- ▶ Ms. Ayushi Mathur (Management)

### Science

- ▶ Ms. Ankita Choudhary (Botany)
- ▶ Ms. Pratibha Sharma (Chemistry)
- ▶ Ms. Monisha Singhal (Biotechnology)
- ▶ Ms. Ritu Kedia (Biotechnology)
- ▶ Ms. Deepika Saxena (Computer Science & IT)
- ▶ Ms. Jaspreet Kaur (Environmental Science)
- ▶ Ms. Parikshana Mathur (Biotechnology)
- ▶ Ms. Anshu Chaturvedi (Home Science)

### NOTIFICATIONS

Workshop on Biotechnology :  
May 16-20, 2022 organised By  
The University of Trans-Disciplinary Health  
Sciences and Technology, Bengaluru

<https://indiabioscience.org/events/whole-genome-and-metagenome-sequencing>

ICEBSER-2022: ICEBSER- International  
Conference on Entrepreneurship, Business  
Studies and Economic Research organized by  
Institute for Educational Research & Development  
(IFERD). Malaysia, June 02, 2022.

<http://iferd.epizy.com/icebser-jun-02-2022/>

18<sup>th</sup> ASIALLICS Conference 2022 (online)  
- Restarting, Innovation and Regional  
Resilience organized by NTHU Institute of  
Technology Management, University of  
Liverpool, Taiwan. June 29-30, 2022

<https://nthu-meetstat.azurewebsites.net/>

9<sup>th</sup> International Conference on Behavioral  
and Social Computing, Organized by Matsuyama  
University, Japan. October 29-31, 2022

<http://besc-conf.org/2022/>

## IISU JOURNALS



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