

# 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



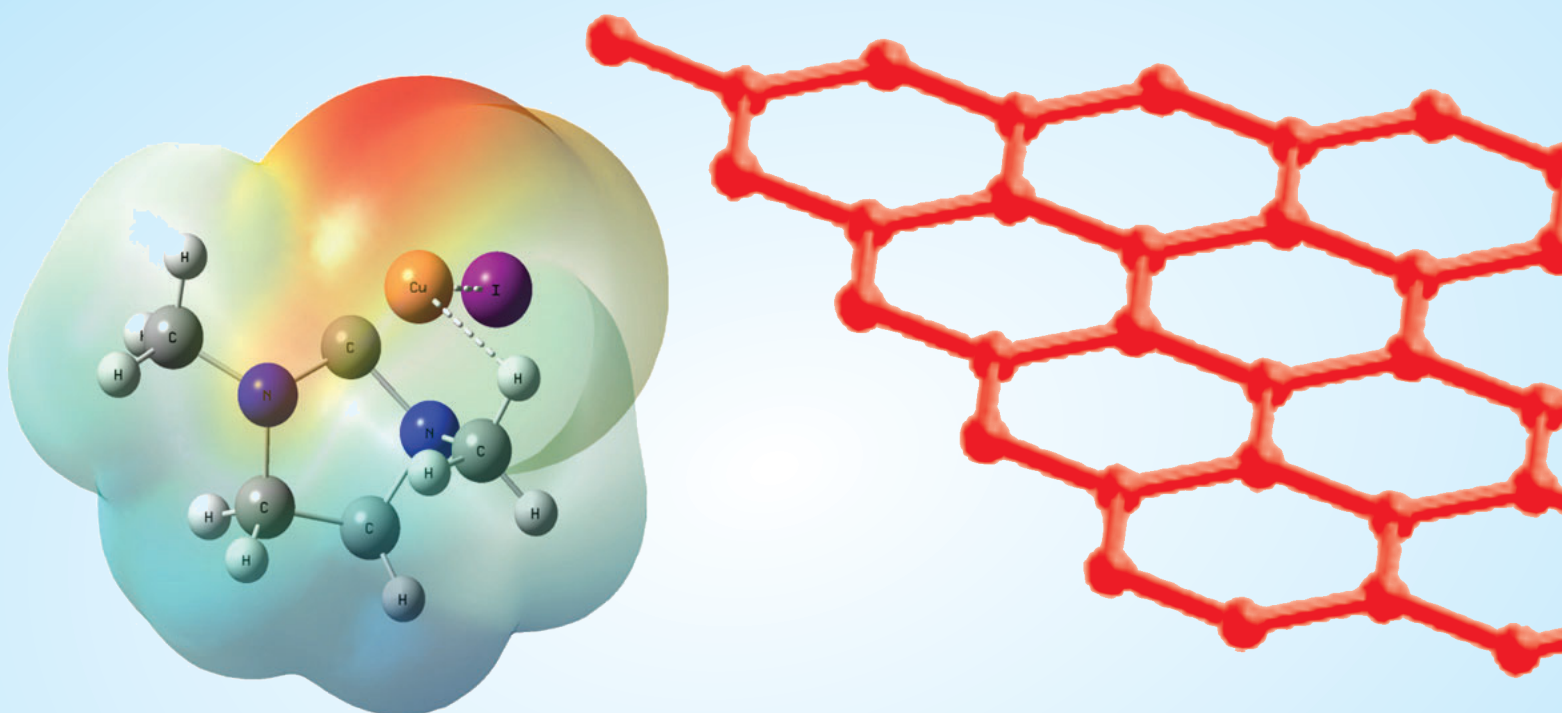
**Centre for Research, Innovation and Training (CRIT)**

IIS (Deemed to be University), Jaipur  
and

**Gramin Mahila Mahavidyalaya, Sikar, Rajasthan**

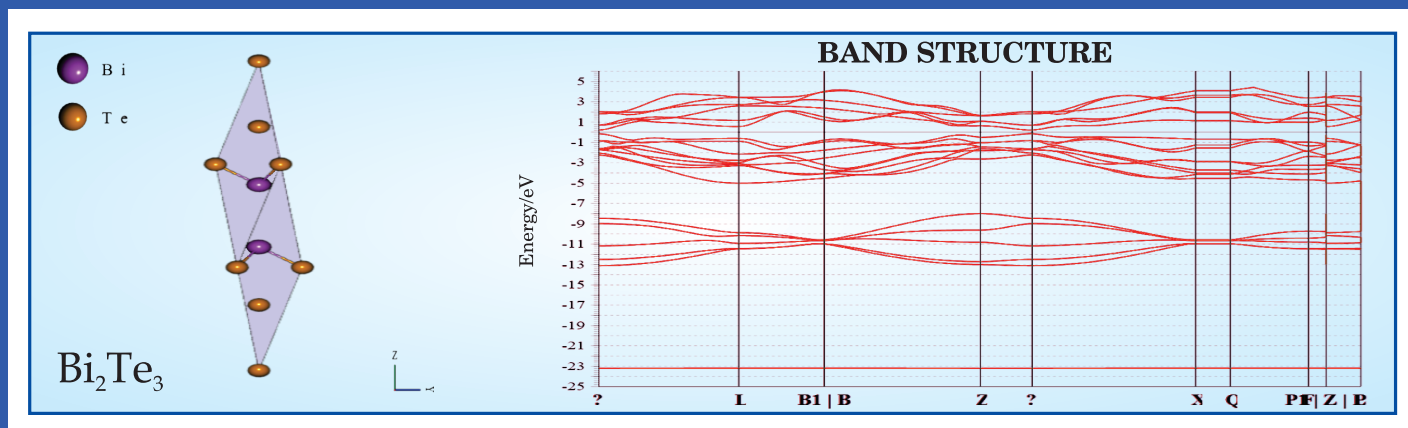


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# ABOUT THE UNIVERSITY

IIS (deemed to be University), Jaipur is among the pioneers in Rajasthan in imparting high quality education to women in different streams. IISU is known for excellence in delivering value-based education to students and encourages them to think innovatively in different walks of life. It particularly focuses on preparing students to become world ready citizens, who are abreast to take any professional and social challenges with an ignited and empowered mind. With over 4500 students, the University offers UG, PG and Doctoral programmes in Arts, Science, Social Sciences, Commerce, Management, Fine Arts, Home Science, Tourism, Advertising, Journalism, Fashion & Jewellery Design and Computer Science & IT etc.



## About the Workshop

The workshop will cover basic concepts as well as some recent advances in computational methods based on density-functional theory for investigation of electronic structure of materials.

Based on DFT, Quantum Espresso has numerous applications, ranging from ground-state energy calculation and structural optimization to molecular dynamics as well as the modeling of structural, electronic and spectroscopic properties. DFT simulations, can be done on any system, like atoms, molecules, compounds and crystalline materials.

Effect of impurities doping on material properties or surface studies can be easily done by using Quantum Espresso (Q.E.). BURAI is a Graphic User Interface (GUI) of Q.E. and enables even the new users to easily investigate materials. The workshop will give exposure of different types of computational codes and will provide opportunity to participants to work on BURAI software to investigate structural and electronic properties of different types of materials.

## Objectives

- To enhance the use of open source software Quantum Espresso and BURAI for Scientific Problems and to promote quality research.
- To help students to give flip to classroom lectures on structure of materials.
- To prepare necessary background for understanding theoretical/computational methods for research in physics and chemistry
- To introduce with the use of other software like WIEN2k and Gaussian.

**ONLINE TRAINING PROGRAMME**

**09 - 17 FEBRUARY 2022**

**2:00 PM - 5:00 PM ALL THE DAYS**

Total Time Duration : 27 hours

## Registration Details

### Target Participants :

UG and PG Students, research scholars and faculty members of Physics and Chemistry disciplines.

### Registration Fees:

Students & Research Scholars : Rs. 500/-

Faculty Members : Rs. 1,000/-

**Last date of registration : 5 Feb, 2022**

### Procedure of registration:

Interested candidates are required to fill online registration form using the link given here.

<https://forms.gle/8gLwXov1sSEqi6Pm8>

Participants are required to submit a soft copy of their University/College IDs and a photograph compulsorily while registering online.

## Important points

- Registration will be done on first come first served basis
- Candidate is required to have his/her own laptop/ desktop with good internet connectivity
- Online platform to be used : Zoom
- Attendance is compulsory in all the sessions to get e-certificate of participation.

### Hardware and Software Required

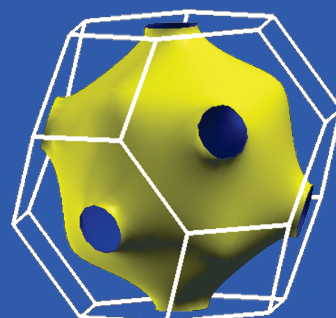
Laptop/Desktop with atleast 4 core CPU and 4 GB RAM, having Java compiler installed and OS Windows 10, with good Internet Connectivity.

## Facilitators/Trainers

- **Prof. P.N. Gajjar**, Head, Deptt. of Physics, University School of Sciences, Gujarat University, Ahmedabad
- **Prof. B.L. Ahuja**, Department of Physics, University College of Science, Mohanlal Sukhadia University, Udaipur (Rajasthan)
- **Dr. C.S. Praveen**, Asstt. Professor, International School of Photonics, Cochin University of Science & Technology, Ernakulam, Cochin (Kerala)
- **Dr. Nandha Kumar**, Brain Pool invited Scientist by the National Research Foundation of Korea, Yonsei University (South Korea)
- **Dr. K.C. Bhamu**, Head, Deptt. of Physics, Gramin Mahila Mahavidyalaya, Sikar, Presently: Senior Post Doctoral Fellow, School of Chemical Engineering, The University of Ulsan, (South Korea)
- **Prof. R.K. Sharma**, Former M.Phil. Coordinator, Maharaja Ganga Singh Univ., Bikaner (Rajasthan)
- **Dr. Shashaank Gupta**, Research Scientist, Virginia Tech India, Chennai (Tamil Nadu)
- **Dr. Smita Sharma**, Associate Professor, Deptt. of Physics, Dungar College, Bikaner

## Facilitators/Trainers from IIS (deemed to be University), Jaipur

- Prof. K.S. Sharma, Director-CRIT and Advisor
- Prof. R.K. Bansal, Professor, Deptt. of Chemistry
- Dr. Varsha Goyal, Associate Professor, Deptt. of Chemistry
- Dr. Trapti Gupta, Associate Professor, Deptt. of Chemistry
- Dr. Rimpay Shukla, Sr. Asstt. Professor, Deptt. of Physics
- Ms. Neeraj Kulhari, Asstt. Professor, Deptt. of Physics





### CHIEF PATRON

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IIS (deemed to be University), Jaipur

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### ADVISORY COMMITTEE

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