

Report of Online 9 Days workshop on D.F.T. investigation of the electronic structure using Quantum Espresso and BURAI Software (Atoms, Molecules, Compounds and Crystalline Materials)

9 -17 February, 2022

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 -17 February, 2022.

The objective of this workshop was to train the participants on the use of DFT, open source software like BURAI and Quantum Espresso. **144** participants were attended the workshop from various reputed institutions of India like IITs, CSIR, University of Delhi, MD University, MLSU, Punjab University, Jiwaji University, the institute of science, MNIT, etc. and other countries like South Korea, Pakistan, etc.

The 9 days workshop comprised of the Inaugural session, 26 technical sessions and the valedictory session.

The inaugural session of the workshop began with welcome address of the Hon'ble Vice Chancellor of the University, Prof. T.N. Mathur. He talked about the basic concepts as well as some recent advances in computational methods based on DFT. Dr. Harshita Garg, Principal, Gramin Mahila Mahavidyalaya, Sikar also welcomed the participants and stressed upon the use of open source software and to promote quality research.

Prof. K.S. Sharma, Director CRIT gave an overview and highlighted the objectives of the Workshop.

Prof. R. K. S. Dhakarey, Hon'ble Vice Chancellor, Maharaja Surajmal Brij University, Bharatpur was the chief guest of the inaugural session to providing his blessings for the success of this workshop.

The Presidential address delivered by the Hon'ble Chancellor of the University, Dr. Ashok Gupta. He stated that this workshop is an attempt to familiarize the participants with the theoretical methods to investigate of different type of materials by using the software Quantum Espresso & Burai.

Keynote address on the topic of "Advanced Density Functional Theory and its Application for band structure calculations in Crystallography" given by Dr. RamphalBrajiram Sharma, Professor & Head Department of Physics, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad (Maharashtra). He was discussed about the fundamentals of density function theory and explained the different theorems and application of DFT for Electronic structure calculation of

materials. Prof Sharma was also explained that how can we use Schrödinger equation for the single and many particle system and approximations to the exchange-correlation functional.

Prof. Raakhi Gupta, Rector and Registrar, IIS (deemed to be University), Jaipur delivered the vote of thanks.

The resource person for I technical session was Prof. R.K. Sharma, Former M.Phil. Coordinator, Maharaja Ganga Singh University, Bikaner (Rajasthan) delivered his talk on “Introduction to Quantum Espresso Input Files & Installation of BURAI”. In his session he introduced the Quantum espresso software and its different tasks. Then he explained about the input files & the Installation of BURAI software on windows 10.

II technical session was taken by Prof. K.S. Sharma on the topic “Fermi Surface”. He focused his talk on basics of quantum espresso software and also performed how we can run the calculations for determining Fermi surface with the help of this.

The day 2 began with III Technical session and the resource person of this session was Dr. C.S. Praveen, Asstt. Professor, International School of Photonics, Cochin University of Science & Technology, Ernakulam, Cochin (Kerala) on the topic “D.F.T.-Introduction and Applications”. He introduced the basic concepts of density functional theory and outlined the features that have lead to its wide applications.

The speaker for technical session IV was Dr. Varsha Goyal, Associate Professor, Deptt. of Chemistry, IIS (Deemed to be University), Jaipur (Rajasthan). She elaborated about the “Electronic Structure of Atoms & Molecules”. She started her talk with the explanation of Atomic structure, Quantum mechanical model of an atom, Schrodinger Wave equation and its solution for hydrogen atom in form of quantum numbers. She beautifully explained the bonding in covalent and ionic compounds, bondorder calculations, energetics of bonding. Finally she ended with the crystal structure of some compounds such as NaCl, ZnO and TiO₂.

The next Technical session V was taken by Dr. Trapti Gupta, Associate Professor, Deptt. of Chemistry, IIS (Deemed to be University), Jaipur (Rajasthan). She gave Hands on Training on Electronic Structure of Atoms using BURAI. In this session they calculated the value of total energy and other important parameters for various atoms using burai software.

Day 3 started with technical session VI taken by Dr. C.S. Praveen on the topic “Revisiting the Landscape of Theoretical Modeling using DFT”. He explained the importance of the exchange-correlation potential for single electron equation and then allied for multi particle system. He also talked about the Hybrid function which gives the better accuracy for DFT calculation.

Next speaker for Technical session 7th was Dr. Trapti Gupta and she gave Hands on Training on Electronic Structure of Linear Molecules using BURAI. This session, is dedicated to the modeling of simple systems such as hydrogen and nitrogen molecules. In this session participants were introduced with the relax calculations to find out the optimized structure of a molecule .

After that next session 8 was taken by me on the topic of Hands on Training on Electronic Structure of Metals (Na) using BURAI. I discussed about the basics of density of states & band structure of metals.

On Day 4 the technical session 9 started with the speaker Dr. K.C. Bhamu, Head, Deptt. of Physics, Gramin Mahila Mahavidyalaya, Sikar Presently at: Senior Post Doctoral Fellow, School of Chemical Engineering, The University of Ulsan (South Korea). He talked about the Checkpoint's of DFT Calculation by taking an example of Silicon using Quantum Espresso Code".

Next speaker for Technical session 10 was Dr. Trapti Gupta and she gave Hands on Training on Electronic Structure of Non-linear Molecules using BURAI. In this session participants learnt to find out the equilibrium structure of non linear molecules such as water and ammonia. She also introduced an excellent tool called Jmol, which they used to find the bond length and bond angle.

Technical session 11 was taken by the resource person Dr. Smita Sharma, Associate Professor, Deptt. of Physics, Dungar College, Bikaner (Rajasthan). She gave Hands on training on Electronic Structure of GaAs using BURAI. She beautifully explained about the convergence processes by using MS excel. She also showed the variations of Ecut off values, K value grid and plotted the respective curves in excel. On basis of these excel curves, she showed the selection of the appropriate value of these parameters.

Day 5 of the workshop was started with technical session 12 & resource person for this session was Dr. SubrahmanyamSappati, Department of Pharmaceutical, Technology and Biochemistry, BioTechMed Center, Gdańsk (gondask),Poland. He gave his talk on Descriptors to predict dye-sensitized semiconductor-based photocatalyst for hydrogen evolution reactions.

Next technical session 13 was taken by Dr. Nandha Kumar, Brain Pool invited Scientist by the National Research Foundation of Korea, Yonsei University, (South Korea).He discussed about Effective Carbon dioxide Utilization Methods: Challenges and Opportunities Affiliation.

After this the next speaker for the session 14 was Prof. R.K. Sharma. He gave Hands on Training on Electronic Structure of Graphene using BURAI. he performed the calculations for geometry,

optimization, band calculations and density of states on BURAI software. For all these processes he explained the input file, run the job followed by the explanation of results.

In session 15 Ms. Neeraj Kulhari, Asstt. Professor, Deptt. of Physics, IIS (Deemed to be University), Jaipur (Raj.) currently working at research scientist, CNR-SPIN, Italy.

Gave Training on Electronic Structure of 2D Material (GeS₂) using BURAI. In this session, she explained in details about Input files (filling of cell, elements and atoms), SCF calculations and output files – Check for convergence, done or not. During the session, she also explained the procedure for downloading the cif file from google, the use of vesta for distance calculation.

On Day 6 the technical Session 16 started with the speaker Dr. Shashaank Gupta, Research Scientist, Virginia Tech India, Chennai (Tamil Nadu). He talked about the “Applications of Quantum Espresso in Advanced Multi-functional Materials”. His talk encouraged participant to actively work in the field of material science using quantum espresso software. He shared his knowledge about how computational tools can help us in determining band gap and electric properties using DFT calculation.

After this session next two technical sessions were taken by Dr. Trapti Gupta & Dr. Smita Sharma gave hands on training on Electronic Structure of Compounds & Topological Insulator respectively by using BURAI.

Day 7 of the workshop was started with technical session 19 & the resource person was Prof. B.L. Ahuja, Department of Physics, University College of Science, Mohanlal Sukhadia University, Udaipur (Rajasthan). The key highlights of this session is use of win2K software for bandgap calculation. This session was indeed an insightful learning experience for all the Participants.

Next speaker for Technical session 20 was Dr. Trapti Gupta and she gave Hands on Training on Electronic Structure of Benzene using BURAI. In this hands on session participants learnt to find the optimized electronic structure of benzene using Burai software. In this session participants were introduced to an excellent tool called molview, which is a modeling and visualization software for molecules that can be loaded in the web browser.

After that in the last technical session of the day Prof. K.S.Sharma gave Hands on Training on Construction of Super Cell & Impurity Doping; Modeling for Surface Studies using BURAI by taking copper element.

Day 8 started with Technical session 22 taken by Prof. Y.K. Vijay, Director-Centre for Innovation in Science Teaching (CIST), IIS (Deemed to be University), Jaipur. (Rajasthan). He discussed about “Measurement of Energy Diagram of an Oscillator using ‘Tracker’ Software”. He explained about measurement of potential energy profile diagram of an oscillator, phase diagram and rocket motion using Tracker software.

In the next technical session 23 I have given Hands on Training on Electronic Structure of TiO₂ using BURAI also discussed about different phases & compared the dos & Band diagram for tetragonal & orthorhombic crystal structure.

In the last session of the day Dr. Trapti Gupta Gave Hands on Trg. on Plotting HOMO and LUMO for Molecules using Quantum Espresso. In this session participants got an idea of performing various calculations such as pdos, charge and homo lumo on quantum espresso in linux environment.

In the last day of workshop technical session 25 started with our resource person Prof. R.K. Bansal, Deptt. of Chemistry, IIS (Deemed to be University), Jaipur(Rajasthan). He focused his talk on “Calculation of Reactivity Descriptors using Gaussian Software”. He discussed various parameters like fukui functions, nucleophilicity, electrophilicity indices and chemical potential.

Last technical session of the workshop was taken by Prof. R.K. Sharma on the topic of Hands on Training on Electronic Structure of Ba-TiO₃ Perovskite using BURAI software.

The sessions were followed by valedictory session.

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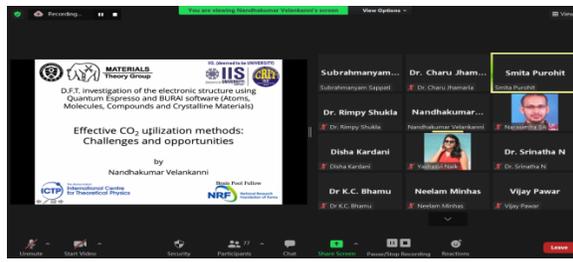
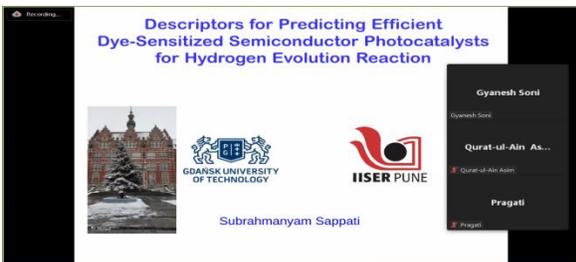
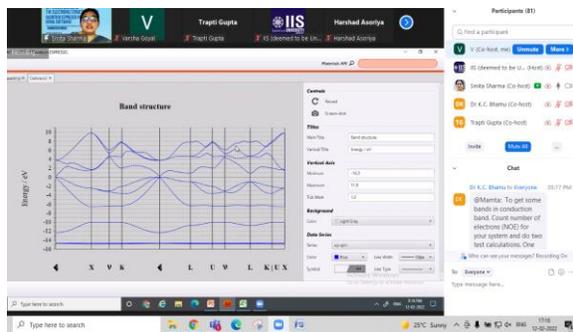
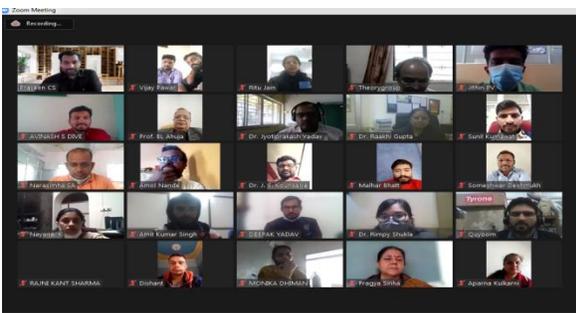
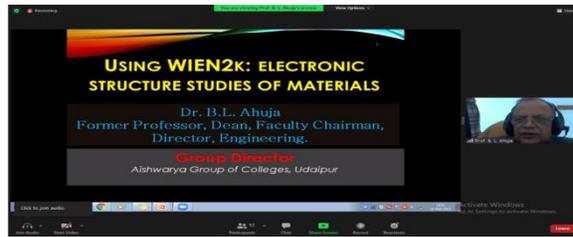
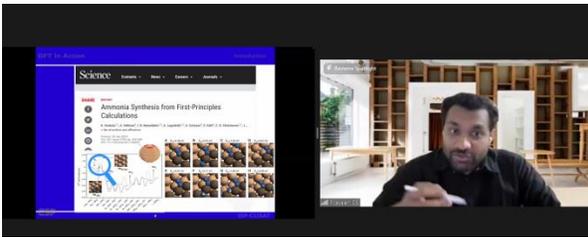
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PHOTOGRAPHS



BROCHURE

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

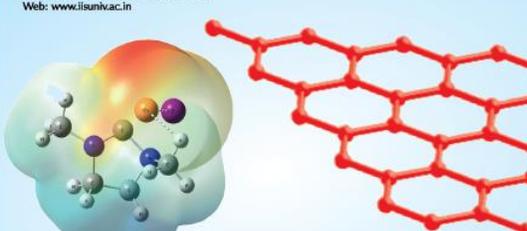
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09 - 17 FEBRUARY, 2022

Jointly Organised by

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

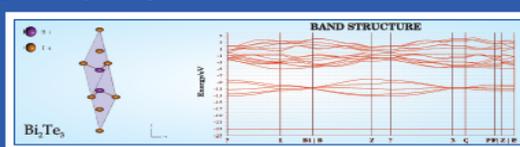
IIS
(deemed to be)
UNIVERSITY
JAIPUR

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Web: www.iisuniv.ac.in



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.



Bi₂Te₃

Band Structure

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/gLwXov1aSEqI6Pm8>
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.

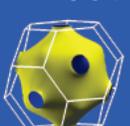
Hardware and Software Required
Laptop/Desktop with atleast 4 core CPU and 4 GB RAM, having Java compiler installed and OS Windows 10, with good Internet Connectivity.

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. Smilta Sharma, Associate Professor, Deptt. of Physics, Dugar 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. Trapiti Gupta, Associate Professor, Deptt. of Chemistry
- Dr. Rimpy Shukla, Sr. Asstt. Professor, Deptt. of Physics
- Ms. Neeraj Kulhari, Asstt. Professor, Deptt. of Physics



CHIEF PATRON
Dr. Ashok Gupta
Chancellor
IIS (deemed to be University), Jaipur

PATRONS

Prof. T. N. Mathur
Vice-Chancellor
IIS (deemed to be University), Jaipur

Prof. Raakhi Gupta
Rector and Registrar
IIS (deemed to be University), Jaipur

ADVISORY COMMITTEE

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Co-Convener
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Head, Deptt. of Physics, Gramin Mahila Mahavidyalaya, Sikar,
Presently: Senior Post Doctoral Fellow, School of Chemical
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ORGANIZING SECRETARIES

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WORKSHOP COORDINATORS

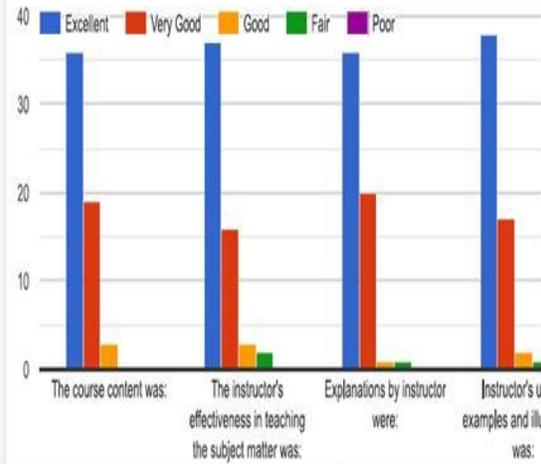
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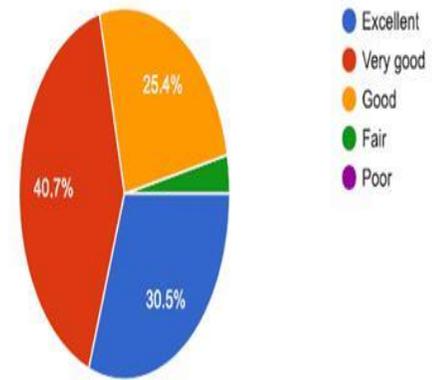


FEEDBACK

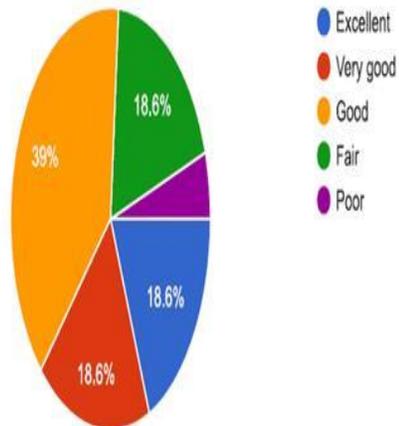
About the session



Learning Enhancement about the topic after attending the session



Knowledge about the topic before attending the session



Learning Enhancement about the topic after attending the session

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