

Report
On
The Workshop
on
**Introductory Methods in
Computational
Chemistry**

2nd April, 2022

Organized by:

Department of Chemistry
in association with
IQAC, Dhemaji College

Submitted by

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Convenor

Department of Chemistry

Dhemaji College

1. Preamble:

A workshop on "Introductory Methods in Computational Chemistry" was organised by Department of Chemistry, Dhemaji College in association with Internal Quality Assurance Cell (IQAC), Dhemaji College on 2nd April, 2022 at Dhemaji College, Dhemaji as an initiative to make the students of UG, PG and Faculties of college aware on the field of computational chemistry.

2. Participant's Profile:

A total of 07 faculties and 94 students were registered for the workshop. The participants were mainly from Dhemaji, Lakhimpur and Tinsukia District.

3. Resource Person's Profile:

Dr. Rahul Kar
Associate Professor
Department of Chemistry
Dibrugarh, Dibrugarh

4. Description about the Program:

In the workshop, Dr. Rahul Kar, Associate Professor, Department of Chemistry, Dibrugarh University as the Resource Person and students and faculty members from 7 colleges of upper Assam took part in the workshop.

The workshop began with the felicitation of honorable Principal Dr Dipak Kr. Neog sir and respected Resource Person Dr. Rahul Kar. A token of appreciation was presented to respected resource person by honorable Principal Sir and Head of Department of Chemistry, Dhemaji College.

This was followed by a welcome address by the Head of Department of Chemistry, Dhemaji College in which he emphasized on the purpose of the workshop to train students and faculty members in the field of computational chemistry.

The inaugural speech was delivered by honorable Principal Sir, Dr Dipak Kr. Neog. He discussed about the importance of computational chemistry in today's era and how it holds great importance in conducting theoretical research. He thanked the honorable Resource person for giving his valuable time to the participants of the workshop.

This was followed by a brief introduction of the honorable Resource person Dr Rahul Kar Sir. Dr Rahul Kar in his talk discussed the importance of computational chemistry in conducting research with special mention for its importance at places where experimental resources are limited. He discussed about the basic of computational chemistry with respect to the DSE course on “Elementary Computational Chemistry” in the 5th semester of CBCS undergraduate curriculum covering Potential Energy Surface, Molecular Coordinate, numerical methods, DFT, Molecular Mechanics etc. An open discussion session between the participants and resource person followed.

Three hands on activity session were conducted in the Department of computer studies of Dhemaji College and the participants were introduced to the use of BASIC, FORTRAN, in computational chemistry. Participants were also introduced to the molecular modeling software Avogadro.

The views of participants were collected at the end in feedback form. Overall a positive and highly encouraging feedback was received from the faculty members and student participants. On receiving the feedback form, certificate of participation was issued to all the participants.

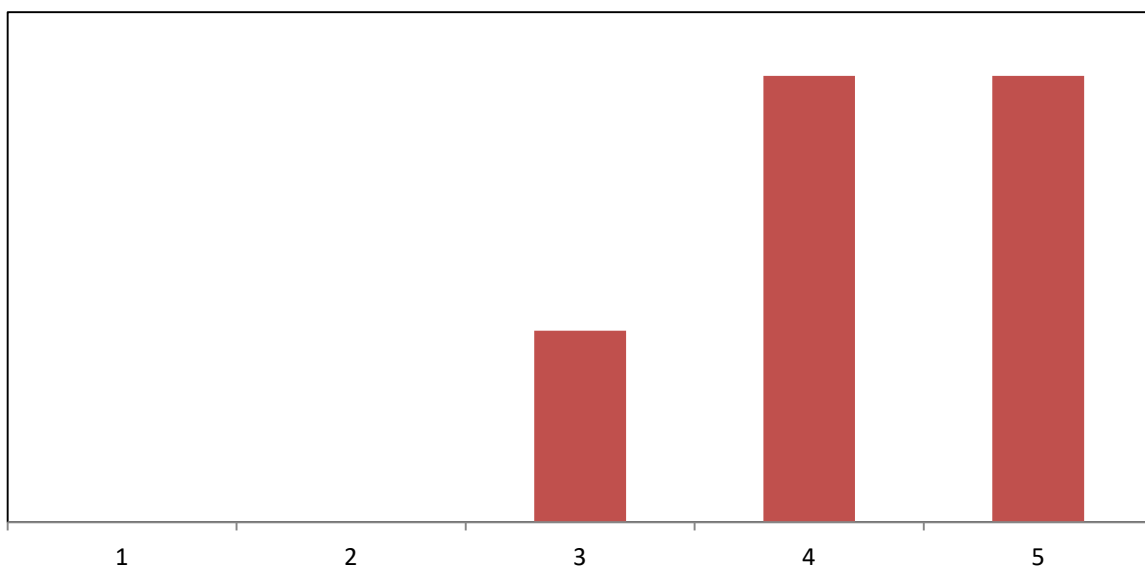
5. Feedback:

Participants expressed their gratitude to the organizing committee for arranging workshop on computational chemistry. Some of the comments are

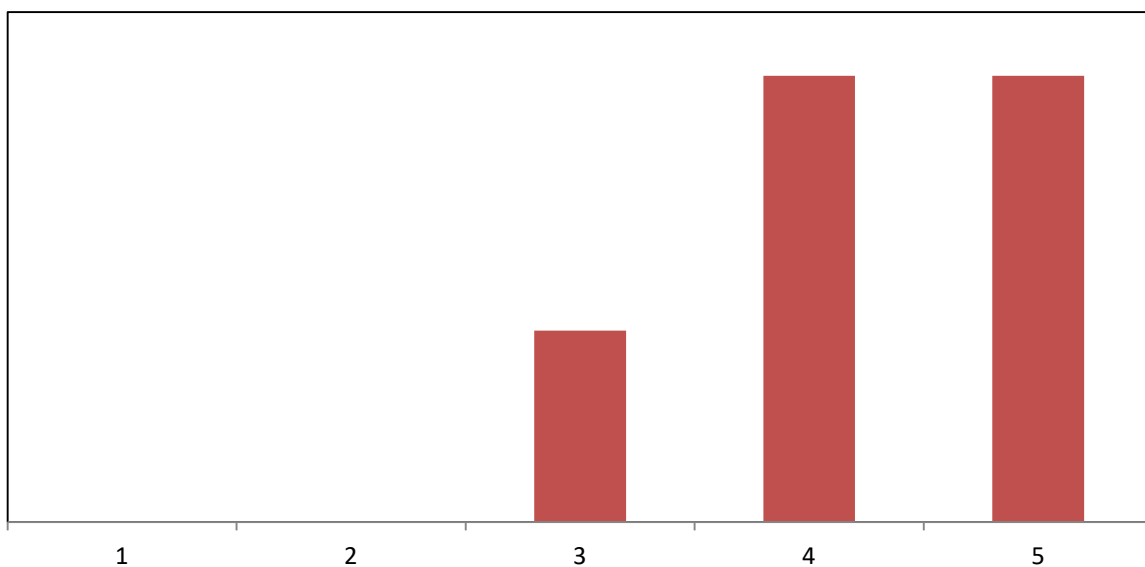
1. Both the sessions are good and informative.
2. 1st session are more informative.
3. Both sessions are relevant.
4. Practical session. As I got to learn so many new things.
5. The technical session was helpful and was very interesting. Thank you.
6. Impressed to hear the lecture and get to know some things.

The graphical representations of the feedback are as follows

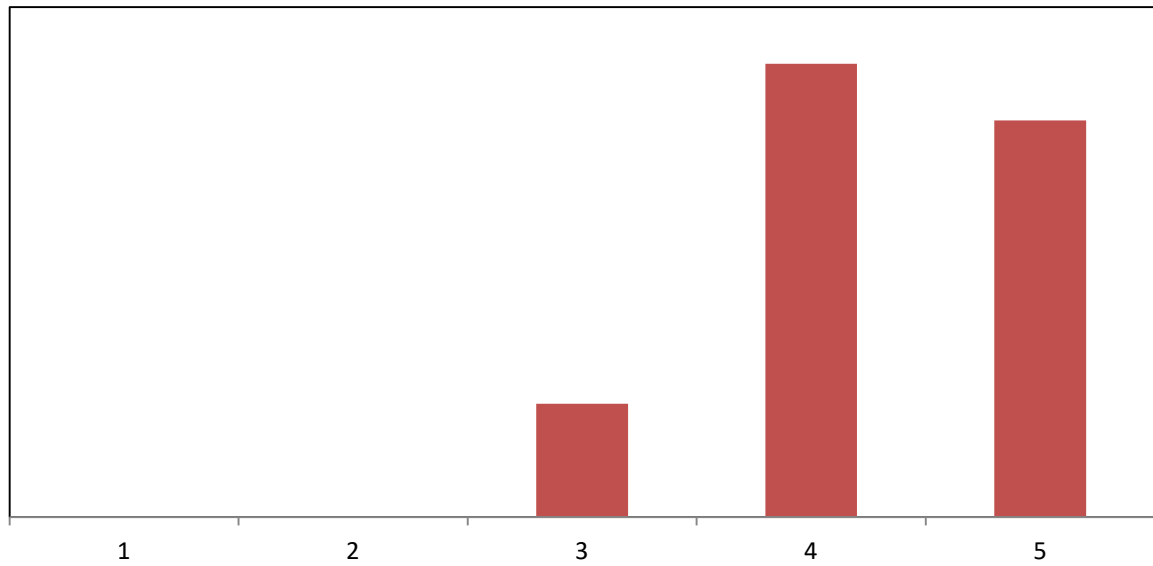
How Much are you satisfied with the events?



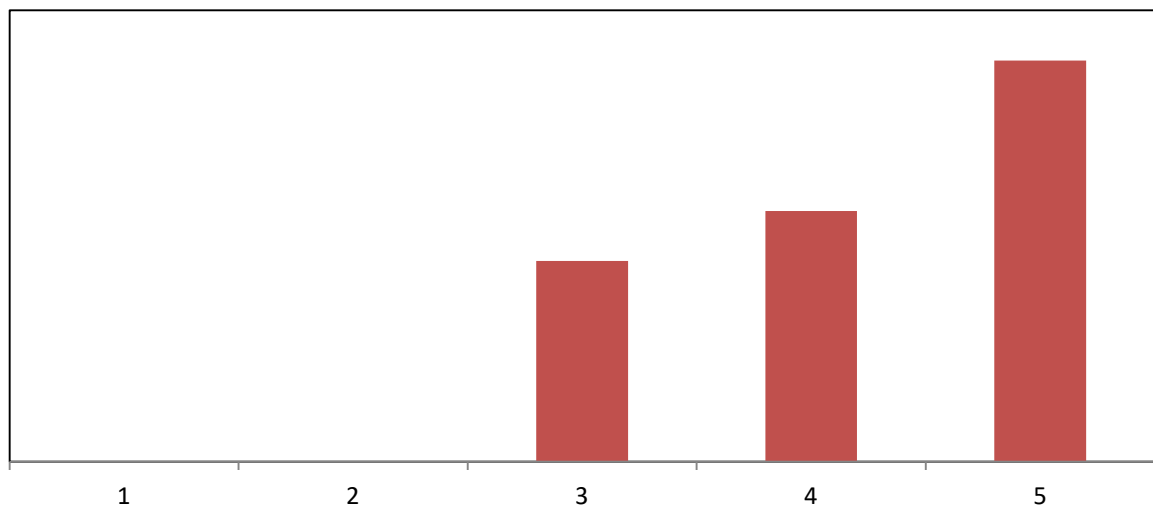
How relevant was the topic for your career?



How much are you satisfied with the organizer?



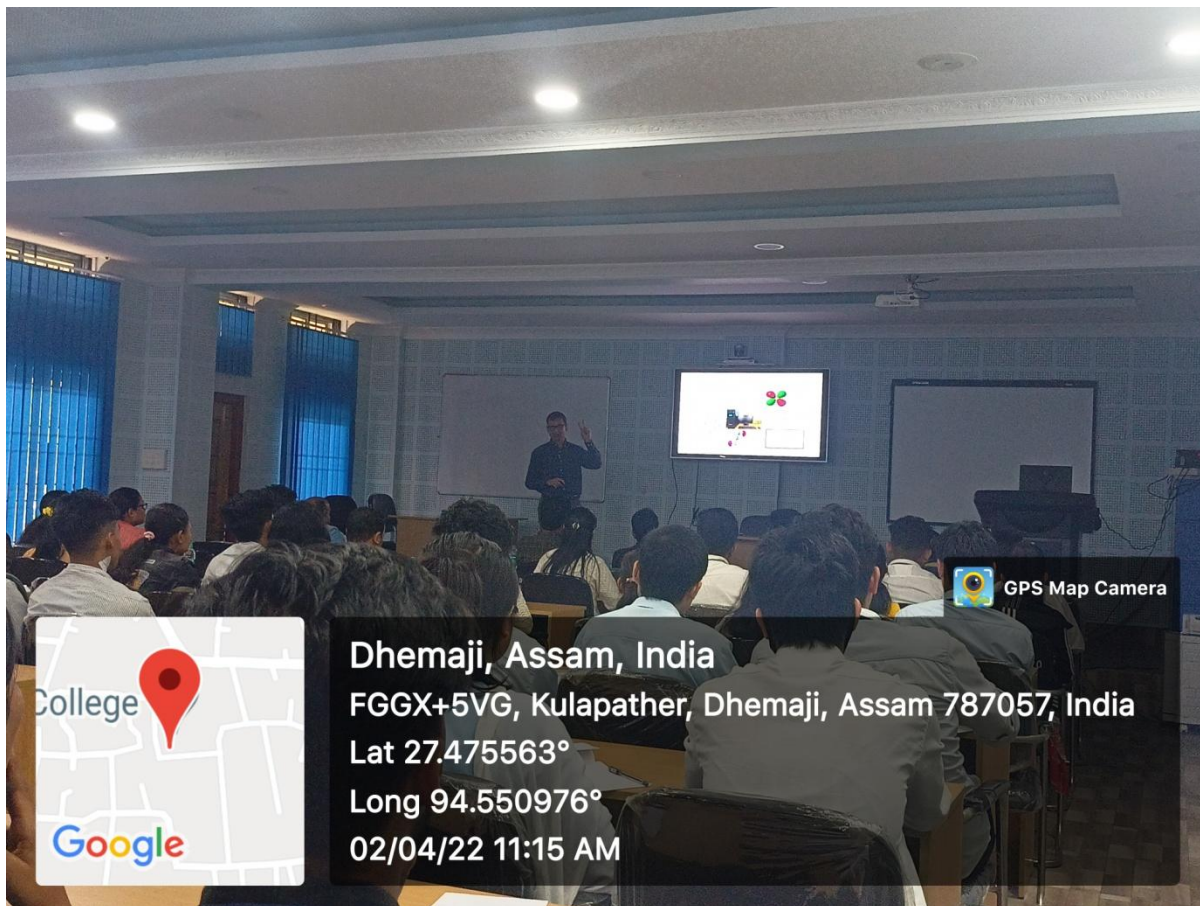
How much are you satisfied with the the session content?

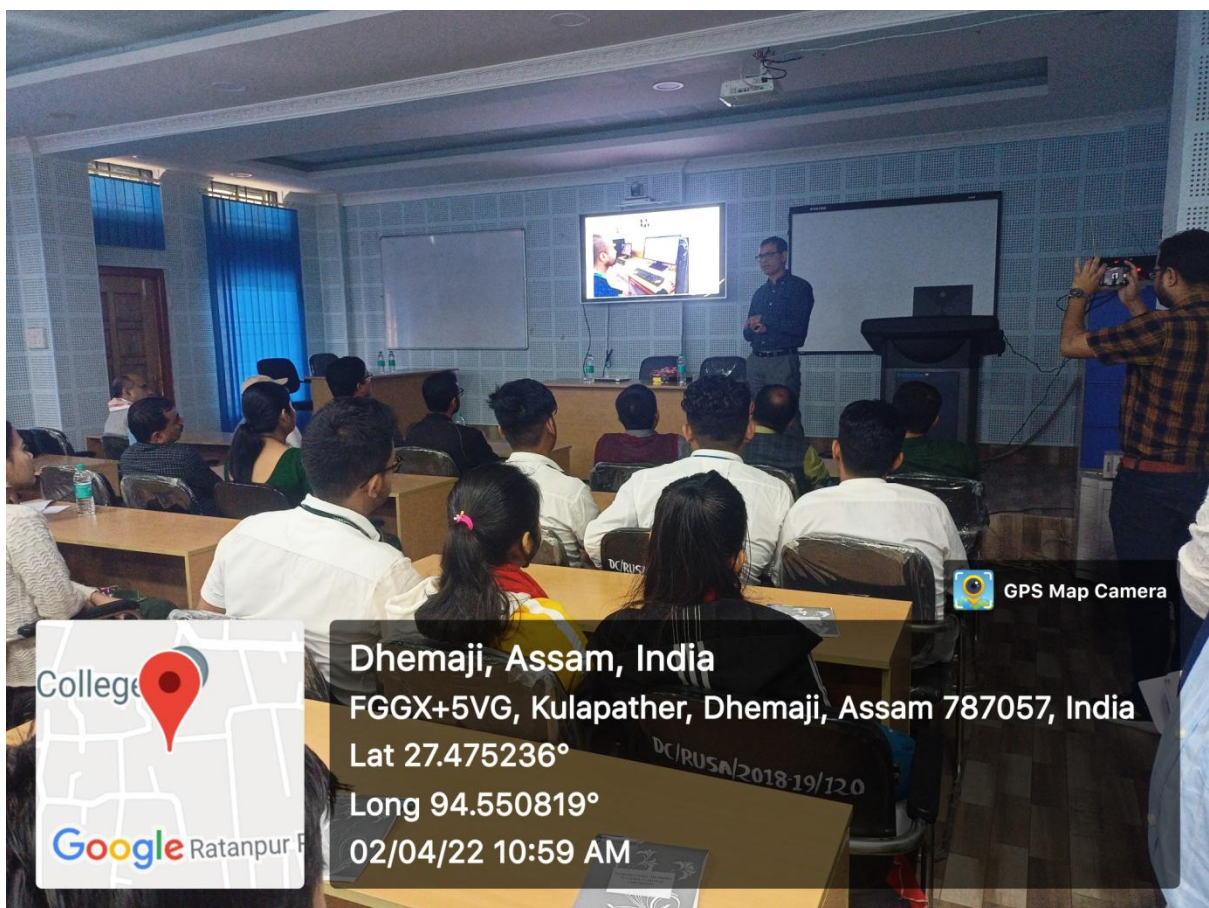
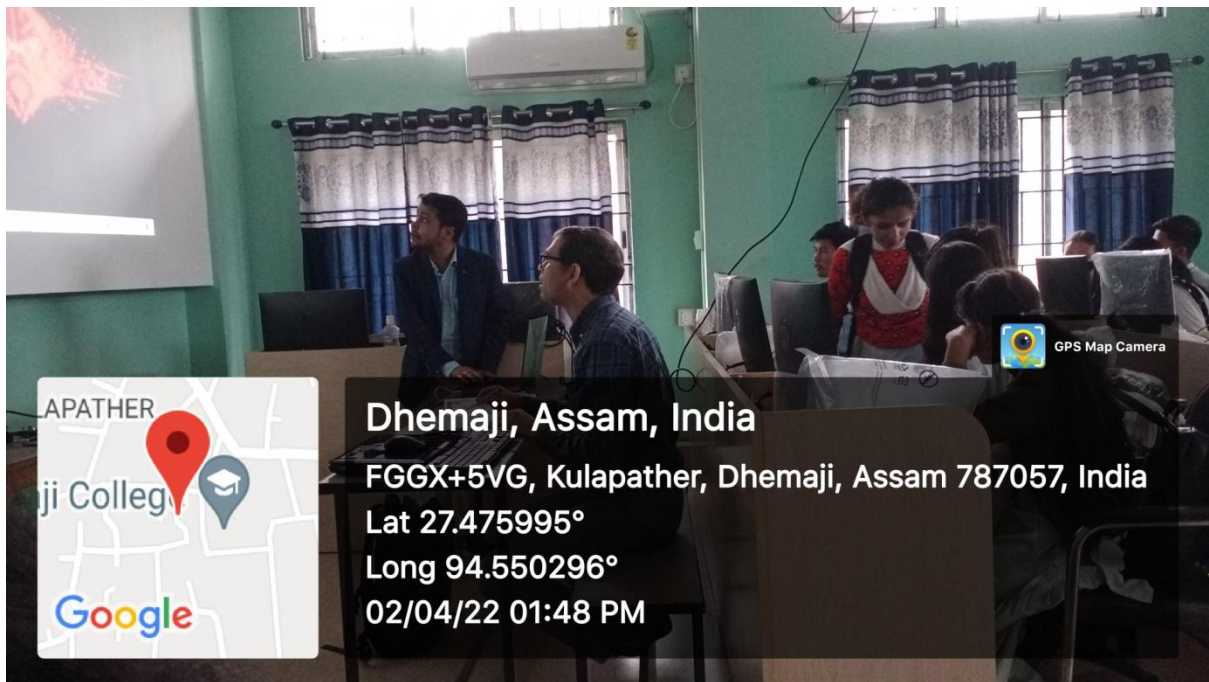


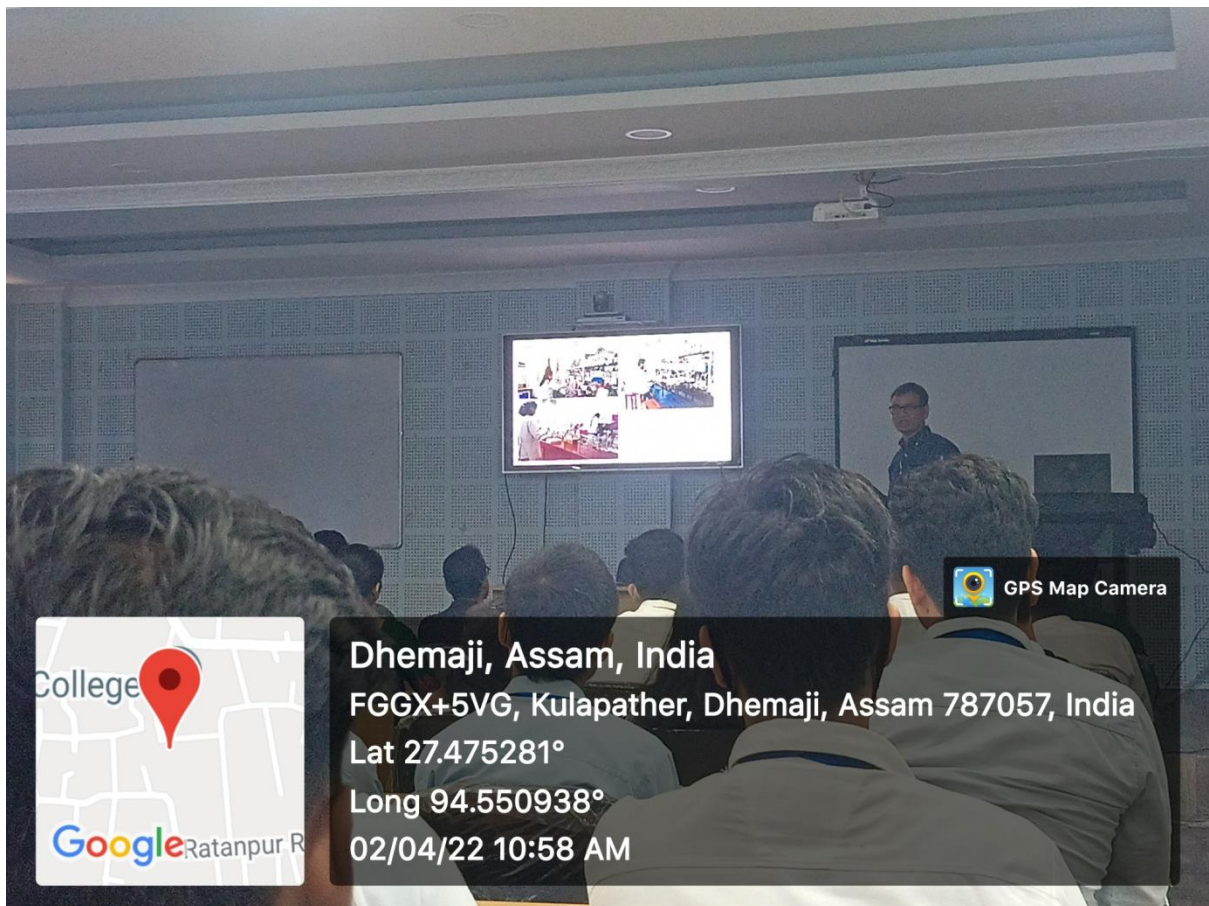
6. Future Perspectives:

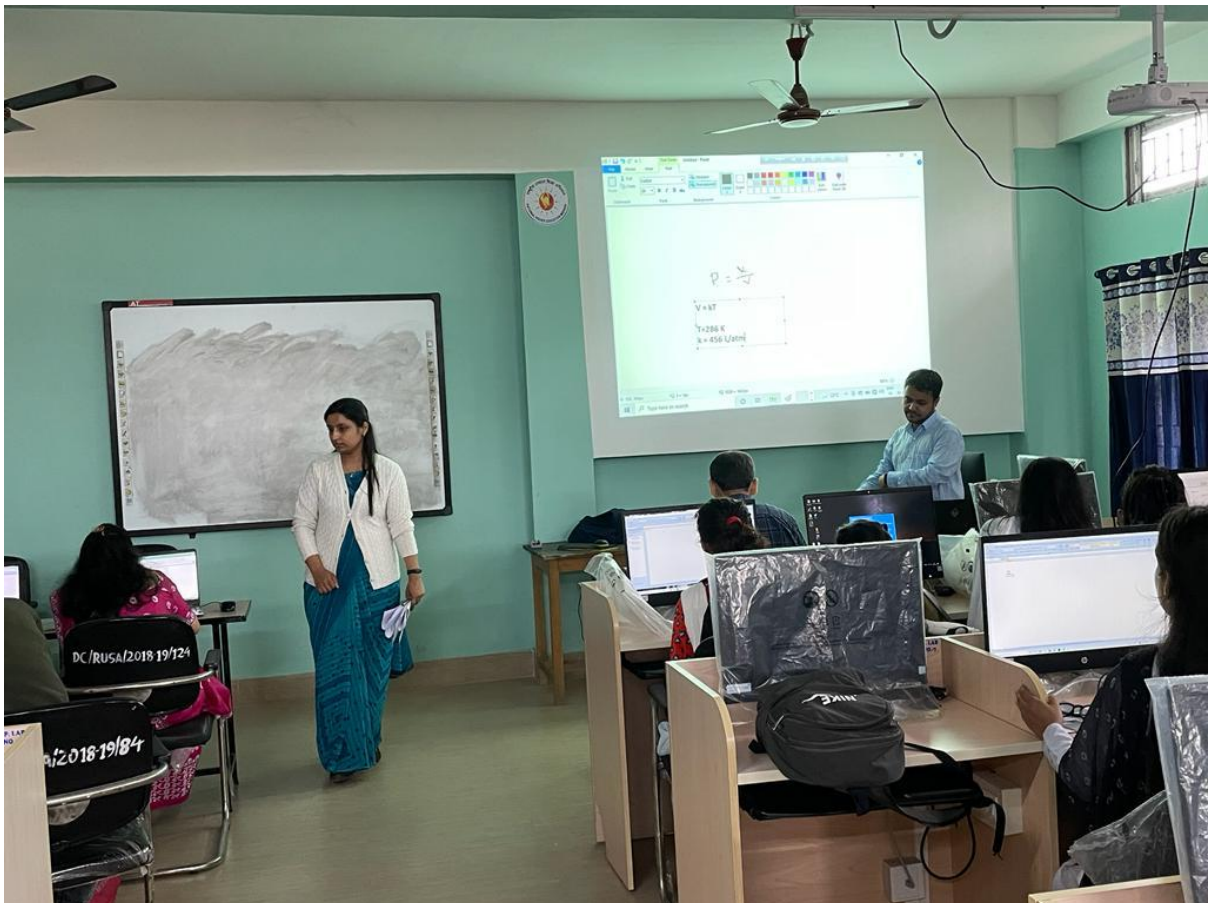
The Department of Chemistry, Dhemaji College looking forward to organize future workshop on computational chemistry in order to increase the knowledge in chemistry among the UG and PG students.

Some Photos of the workshop













Dr Manash Protim Borpuzari
Convenor