

Report of the Three-Days Online Workshop on
"Computational Designing of Molecules and Materials"

August 14 -16, 2021

Jointly organized by-



Department of Chemistry & Department of Botany

Government PG College, Berinag, Pithoragarh
Uttarakhand, India -262531

Patron:

Prof. C D Suntha
Principal
Government PG College, Berinag

Coordinators:

Dr. P C Mathpal
Assistant Professor
Department of Mathematics
Government PG College, Berinag

Dr. Ankita Joshi
Assistant Professor
Department of Chemistry
Government PG College, Berinag

Mr. Ashwini Kumar
Assistant Professor
Department of Botany
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Dr. B S Bisht
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Dr. Beena Lohiya
Assistant Professor
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Government PG College, Berinag

Report of the Three-Days Online Workshop on "Computational Designing of Molecules and Materials"

A three days Online Workshop on "Computational Designing of Molecules and Materials" was held in Government PG College, Berinag on August 14 - 16, 2021 via Google Meet platform. The workshop was jointly organized by Department of Chemistry and Department of Botany, Government PG College, Berinag. Dr. Ankita Joshi, Assistant Professor, Department of Chemistry was the moderator as well as the coordinator of the workshop. The entire program was coordinated with the support of Dr. P C Mathpal, Mr. Ashwani Kumar, Dr. B S Bisht and Dr. Beena Lohiya.

The workshop had altogether six sessions. Researchers from various distinguished institutions were invited to deliver lectures on importance of computational designing of novel molecules and materials using computational methods. The workshop was envisioned to have the insight of the basic software packages and exposure of advanced techniques in the field of research. About 75 participants (undergraduate, postgraduate students, research scholars, faculty) from various institutions participated in this three days online workshop.

The following team of researchers enlightened the participants by their lectures.

1. Rameshwar L. Kumawat, *PhD*, Department of Chemistry, IIT Indore
2. Shyama C. Mandal, *PhD*, Department of Chemistry, IIT Indore
3. Diptendu Roy, *PhD*, Department of Chemistry, IIT Indore
4. Akhil S. Nair, *PhD*, Department of Chemistry, IIT Indore
5. Jai Krishna Mahto, *PhD*, Department of Biotechnology, IIT Roorkee
6. Kumud Pandav, *PhD*, Department of Biotechnology, IIT Roorkee

The three days workshop was inaugurated on 14th August 2021 by our Patron Prof. C D Suntha, Principal Government PG College, Berinag. Prof. Suntha, during his Presidential address, welcomed all the participants joining from different colleges of the state. The coordinator of the workshop, Dr. Ankita Joshi highlighted the theme of the workshop and briefed about the lecture series to be followed. The following lectures were delivered during the workshop:

Day/Date	Time	Topic	Presenter
Saturday August, 14	2-3 pm	SIESTA and TranSIESTA Technical Presentation for the Structural, Electronic and Transport Studies	Rameshwar L. Kumawat
Saturday August, 14	3-4 pm	Understanding the Material World from Computational Perspective	Akhil S. Nair
Sunday August, 15	2-3 pm	Basic Understanding of Machine Learning	Diptendu Roy
Sunday August, 15	3-4 pm	Computational biology in drug discovery: application perspective	Jai Krishna Mahto
Monday August, 16	2-3 pm	Introduction to Autodock, Pymol and VMD Tools	Kumud Pandav
Monday August, 16	3-4 pm	Basic Computational Techniques for Molecular Designing and Applications	Shyama C. Mandal

The entire sessions were interactive and the speakers answered many queries raised by the participants.

In the feedback session, the young and energetic participants from various institutions expressed their views about the workshop. They appreciated the coordinator for the well organized workshop and also suggested the department to conduct more workshops and seminars in the years to come.

The three days workshop ended with the valedictory address by our Principal sir Prof. C D Suntha.

Photographs:

Computationally Designing of Molecules and Materials
IIT Indore

SIESTA/TranSIESTA Technical Presentation
(Structural, Electronic, Transport, Magnetic, Optical etc.)

Rameshwar Lal Kumawat (PhD)
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Department of Metallurgy Engineering & Materials Science
Department of Chemistry

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People: ashwin kumar (You), Aarti Tanta, ANGAT DHAMAN, Anjal Dhanki, Anika Joshi, Babita Sangari, Dr. Leet Singh, Dr. prakash mathpal, Dr. Prathiba Nagi, garga rawat

Autodock, PyMol and VMD

Kumud Pandey
Department of Biotechnology
Indian Institute of Technology Roorkee

People: Anika Joshi, SHYAMA MANDAL, Mamd Panti, Babita Sangari, Anika Joshi, Kumud Pandey, Manbeer Kandi, 18 others

Schrodinger Equation: Pillar of first principles methods

Erwin Schrodinger

$$\hat{H}\Psi = E\Psi$$

$\Psi_{total} = \Psi_{el} \Psi_{nu} = \frac{1}{\sqrt{N!}} \left(\prod_{i=1}^N \psi_i \right) e^{-i\mathbf{r} \cdot \mathbf{p}}$

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11 atomic wavefunctions
11 atomic orbitals

People: ANKIT S, ANKIT Presentation, ANGAT DHAMAN, Anjal Dhanki, Anika Joshi, Babita Sangari, CHANDRA DATT SUNTHA, Dipendu Roy, Dipendu Roy, Durga Prasad, Gargya bantoli

Why Computational Chemistry?

Transition state Z, Intermediate Y, Intermediate X

A = B → C

Favorable or not?

Questions:
Reaction will be happen or not?
If happen
What will be the required environment?
What will be the intermediates?
What will be the transition states?

Time
Cost
Effort
Unknown facts
Pathways
Explanation

People: SHYAMA MANDAL, Anika Joshi, Kumud Pandey, ADARSH KUMAR, 18 others, You

Basic understanding of Machine Learning

PRESENTED BY
DIPENDU ROY

People: ANKITA JOSHI, Dr. Sakun Singh Bisht, Dr. prakash mathpal, Anjal Dhanki, Dipendu Roy, beena lohya, Jai Krishna, 12 others

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

Computational biology in drug discovery: application perspective

Presented by:
Jai Krishna Malvi
IIT Roorkee, Roorkee

People: Jai Krishna, Jai Krishna Presentation, Jyoti Dhanki, Fajar Panti, Kalyani Joshi, Manisha Saradoti Menon, Manbeer Kandi, Manvi, natia ghoshal, Neha KATHARAT, Pooja Upadhyay, Rameshwar Lal Kumawat