



FDP on "Material Studio"

Organized By

Centurion University of Technology and

Management Date: 24-05-2021 to 15-06-2021

No. of Participants:

33 Resource Person

Dr. Padmaja Patnaik, Associate Professor in School of Applied Sciences, Department of Physics has done her PhD in Physics from IITB, Mumbai under the guidance of Dr Gautam Mukhopadhyaya and Dr Prabhakar P Singh of IITB, Mumbai. She focuses on the application of theory behind many scientific research and applications in the field of Physics and Material Science to solve modern day problems and foster innovation at grass root and industry levels. She has published a book and papers in the field of Condensed Matter of Physics and currently she and her team are actively researching in this area

About the session:

From Introduction to Molecular Modelling to studying zeolites for adsorption of gas molecules, the five-day workshop dealt with various topics.

Designed and led by: Dr. Yamini Sistla

The Biovia Materials Studio Workshop organised over 5 days in November 2020, saw keen participation from 16 students belonging to different departments. The workshop addressed a range of pertinent topics during each of the 1.5 hour session slots across 5 sessions.

Session 1 10 am to 11am

Introduction to Molecular Modelling
Introduction to Material Studio

Session 2 11am to 1pm

Building molecular structures, polymers, surfaces & layers

Session 3 1pm to 3pm

Building molecular structures, polymers, surfaces
Modelling of single molecules using quantum mechanical approach and analysis (Modules to be used: Molecule builder, DMol3, CASTEP)

Computing density of liquids (Modules to be used: molecular sketch, DMol3, amorphous cell, Forcite)

Session 4 3pm to 4pm

Conformer structures study (Modules used: molecular sketch, DMol3, Conformers)

Gas diffusivity (Modules used: molecular sketch, DMol3, amorphous cell, Forcite)

Computing glass transition temperature, melting point, boiling point (Modules to be used: molecular sketch, DMol3, amorphous cell, Forcite)

Session 5 4pm to 6.15pm

Studying zeolites for adsorption of gas molecules (Modules to be used: Molecule builder, CASTEP, adsorption locator)

Adsorption isotherm of gas molecule on polymer (Modules to be used: Molecule & polymer builder, DMol3, Amorphous cell, Forcite, Sorption)



WorkShop on Material Studio

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Sciences, Department of Physics

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Brochure of the event



NO. of Participants

1	Dr.Aswini Kumar Rath	Prof. Dept. of Botany
2	Mrs.Namita Panda	Asst.Prof
3	Dr.Jyoti Prakash Rath	Asst.Prof
4	Dr.Shanatanu Bhattacharya	Asst.Prof & HOD, Dept. of Botany
5	Dr.Pratibha Rani Deep	Asst.Prof
6	Mr. Debashish Tripathy	Asst.Prof & HOD, Dept. of Zoology
7	Mr.Pankaj Meher	Asst.Prof
8	Mr.Sujit Kumar Mishra	Asst.Prof
9	Mr.Chinmayee Tripathy	Asst.Prof
10	Swapna nanda Rath	Professor

11	G. N. Inndresha	Professor
12	Firoz Ahmed	Professor
13	Dr.Aditya Kumar Purohit	Asst.Prof
14	Dr.Srikanta Moharana	Asst.Prof
15	Dr.Ashish Kumar Sarangi	Asst.Prof
16	Mr.Rajguru Rajesh Raman Mishra	Asst.Prof
17	Dr.Bhairaba Kumar Majhi	Asst.Prof & HOD, Dept. Of Mathematics
18	Mr.Satyabrata Sadangi	Asst.Prof
19	Dr.Jayakishan Meher	Prof. & HOD, Dept. Of IT & BCA
20	Mrs.Monalisha Joshi	Asst.Prof
21	Ms. Asharani Dalei	Asst. Prof
22	Dr.Nilaya Kumar Mohanty	Asst.Prof & HOD,Dept Physics
23	Mr.Gyanendra Kumar Mishra	Asst.Prof
24	Mrs.Meena Kumari Sahu	Asst.Prof
25	Mrs.Sasmita Pradhan	Asst.Prof
26	Dr. Prafulla Kumar Sahu	Prof.
27	Mr.Vijaya Kumar Meher	Asst.Prof
28	Mr. Dinesh Kumar Sharma	Asst.Prof
29	Mr.Ashish Kumar Meher	Asst.Prof
30	Mrs.Binapani Barik	Asst.Prof
31	Mr. Biswajeet Acharya	Asst.Prof
32	Mr.Swarnajeet Tripathy	Asst.Prof



Dr. Prasanta Ku. Mohanty
Dean Academic



Prabhat K. Pattnaik
FDP Coordinator