

POSTGRADUATE AND RESEARCH DEPARTMENT OF CHEMISTRY

VIVEKANANDA COLLEGE

STUDENT DEVELOPMENT PROGRAMME

ON

COMPUTATIONAL CHEMISTRY (Under DBT Star College Scheme)

21st July 2022, Thursday

Postgraduate & Research Department of Chemistry



Vivekananda College

*(Residential & Autonomous – A Gurukula Institute of Life-Training)
College with Potential for Excellence
Re-accredited with 'A' Grade (CGPA 3.59 out of 4.00) by NAAC
Affiliated to Madurai Kamaraj University,
Tiruvedakam West – 625 234, Madurai, Tamil Nadu*



**Student Development Programme on
Computational Chemistry
(under DBT Star College Scheme)**

Swami Vedananda

Secretary

Swami Adhyatmananda

Kulapathy

Dr.T. Venkatesan

Principal

Dr.G.Ponraj

**Coordinator,
DBT STAR College Scheme**

Mr.B. Servaramuthu

**Head and Dept. Coordinator
DBT STAR College Scheme**

Dr.G.Rajkumar

Convenor

Dr.A.Kannan

Organizing Secretary

Sri.A. Dharmanandham

Treasurer

Members:

Dr.M.Ganapathi

Sri.M.Ragu

Dr.D. Thirupathi

Dr.G. Balakrishnan

Dr.S. Ellairaja

Lecture 1: 9.45 – 11.15 am

Date: 21.07.2022

Dr.S.S. Syed Abuthahir

Assistant Professor of Chemistry

Jamal Mohamed College (Autonomous)

Trichy - 620 020

**Title: Basic Features, Tools and Interpretation of
Chemical Structures using ChemDraw Software**

Lecture 2: 11.30 am – 1.00 pm

Dr.S.S. Syed Abuthahir

Assistant Professor of Chemistry

Jamal Mohamed College (Autonomous)

Trichy - 620 020

Title: Hands-on-training on ChemDraw Software

Lecture 3: 2.00 – 3.30 pm

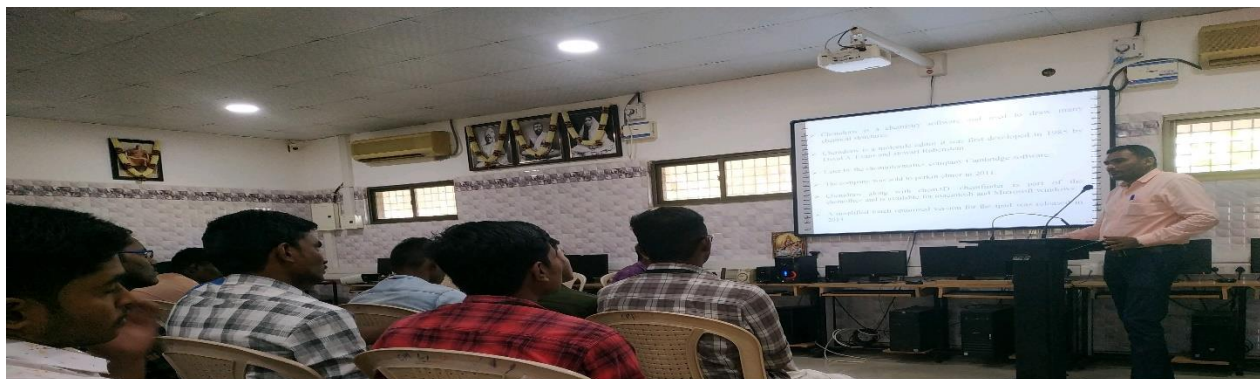
Dr.A. Kosiha

Assistant Professor of Chemistry

**Vels Institute of Science, Technology & Advanced
Studies (Deemed to be University)**

Chennai - 600 117

Title: DFT Calculations using Gaussian Software



Unnamed Road, Tamil Nadu 625214, India

Tamil Nadu
India

2022-07-21(Thu) 10:39(AM)

33°C
91°F

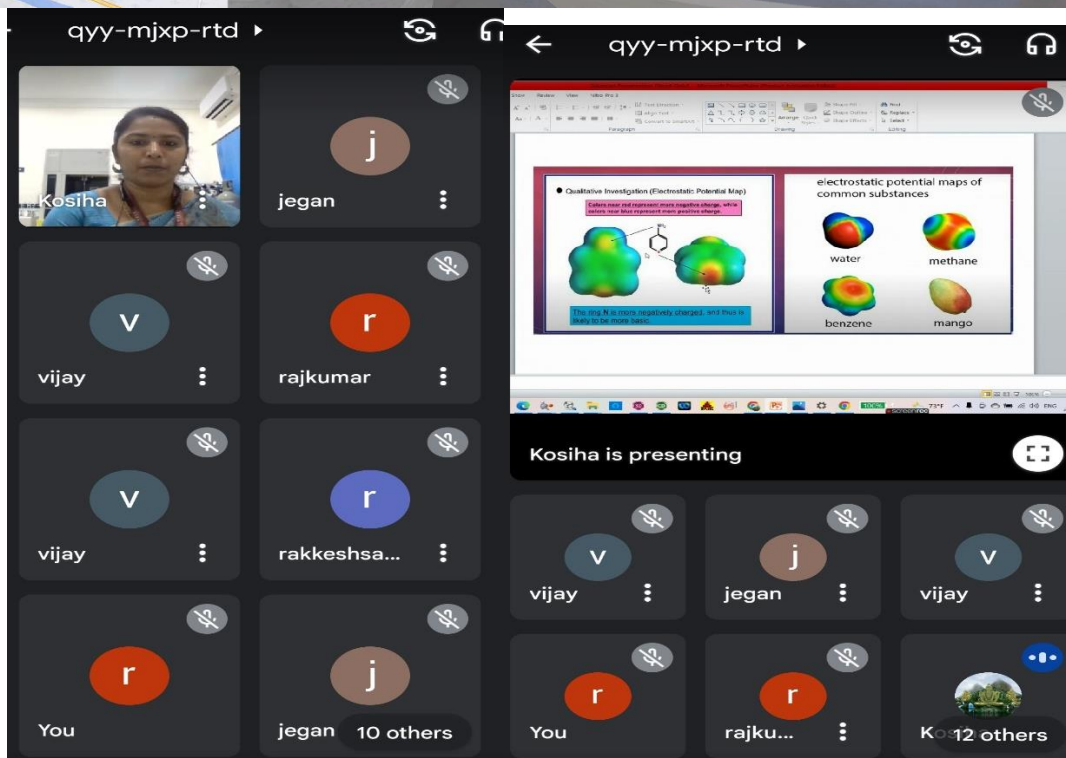


Unnamed Road, Tamil Nadu 625214, India

Tamil Nadu
India

2022-07-21(Thu) 03:46(PM)

36°C
97°F



Report:

A student development programme on “**Computational Chemistry**” under DBT Star College Scheme was organised on 21st July 2022, Thursday by Postgraduate and Research Department of Chemistry, Vivekananda College, Tiruvedakam West. Dr.G.Rajkumar and Dr.A.Kannan, convenor and organizing secretary respectively, scheduled this programme. The Inaugural session commenced at 9.40 a.m. with prayer “*Om Sahanavavathu*” followed by welcoming the gathering by Sri.B.Servaramuthu, Head and Assistant professor of Chemistry. The presidential address was given by Dr.T.Venkatesan, Principal of our college. Dr.G. Ponraj, Associate Professor of Zoology, Coordinator of DBT STAR College Scheme gave the felicitation address. The treasurer of this SDP programme Sri.A.Dharmanandam proposed the vote of thanks for the inaugural function.

The technical session commenced at 10.00 am by Dr.S.S. Syed Abuthahir, Assistant Professor of Chemistry, Jamal Mohamed College, Trichy on the title “Basic Features, Tools and Interpretation of Chemical Structures using ChemDraw Software”. He explained the basic tools and how to draw the chemical structures using ChemDraw software. His lecture was highly informative and beneficial which we interpreted from active participation of students.

The technical session II at 2.00 pm was given by Dr.A Kosiha, Assistant Professor of Chemistry, Vels Institute of Science, Technology Advanced Studies (Deemed to be University), Chennai on the title “DFT Calculations using Gaussian Software” through GoogleMeet. She explained the calculation of HOMO, LUMO, global softness, hardness etc values using Gaussian software. The theoretical interactions between molecules were explained by the resource person. The SDP programme ended with prayer “Sarve Bhavanthu”.