Two Days National Level Work Shop on

Introduction to Molecular Modelling-Report

17th and 18th June 2021

Online Platform-Zoom

Resource Person : **Dr. L. Akilandeshwari**
Assistant Professor in Chemistry,
Sri Sarada College for Women, Salem

Dr. S. AnbuSelvi
Assistant Professor in Chemistry,
Sri Sarada College for Women, Salem

Programme Co-ordinator: **Dr. M. Malarvizhi,**
Assistant Professor and Head
Department of Chemistry

No. of Participants : **265**

Registration Link:

https://forms.gle/UHzFjm2hAd4RFfEe6

Feed Back Form Day 1:

https://forms.gle/Gko3A9YhGrr3sJxK9

Feed Back Form Day 2:

https://forms.gle/2Cry6vEM8k2vswEY9

Assignment Link:

https://forms.gle/BnCtdRq1MrP6UkFT8

You Tube Video links

http://www.youtube.com/watch?v=bAOTbZaq85k

https://youtu.be/H4JEXq7aNkg

Chemistry isn't what it used to be. There was a time when things were, some might argue, simpler. It was practical, wet, occasionally dirty and sometimes smelly. Now, a large group of chemists are exchanging the 8-hour lab sessions for screen marathons, not working with chemicals but simulating them. The rise of molecular modelling is changing the face of chemistry in exciting new ways, which could present both opportunities and challenges to the chemical sciences as a whole and to chemistry education.

Molecular modelling has been called the fourth axis of chemistry – it lies somewhere between theory, observation and experiment. At its core are attempts to describe the state and behaviour of molecules through computer simulations – a fundamentally different approach

to the rest of chemistry. For Carmen Domene, a computational chemist at King's College London, it is also a way to see chemistry from a completely new angle.

The scenario of the industry has changed drastically over years and in the present times, the industrial skills demanded from students cannot be gained merely by academic courses. In such situations, various workshops play an imperative role in bridging this gap and enable the students to acquire industry-relevant skills.

Chemistry Department of Sri GVG Visalakshi College for Women, Udumalpet has conducted different online workshops during time of the Covid-19 pandemic to assist students to develop skills and expertise in interesting fields without any hindrance.

The 2-day workshop on **Molecular Modelling** was successfully conducted on 17.06.2021 and 18.06.2021. The workshop aimed at equipping young students and researchers with essential knowledge of various molecular modelling techniques.The objective of the workshop is to develop skills in molecular dynamics and to enrich knack in structural and comparative analysis.

Invitation

Day 1:

The workshop commenced with the inauguration ceremony. Dr.M.Malarvizhi, Head,Department of Chemistry welcomed the gathering. Dr.N.Rajeswari, Principal of the

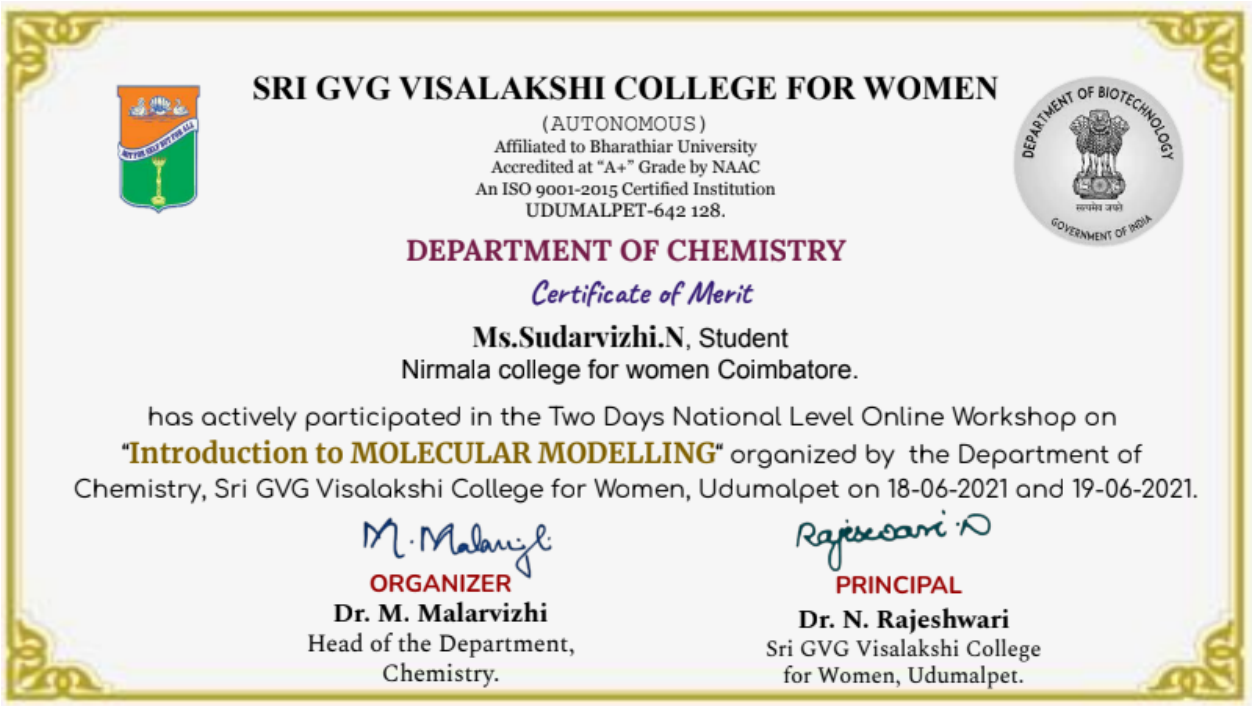
College in her felicitation address congratulated the team for organizing this sort of workshop which is need of the hour and she also greeted the resource speakers and the participants.

As the first Resource speaker, **Dr. L. Akilandeshwari, Assistant Professor in Chemistry, Sri Sarada College for Women, Salem**was introduced. The resource person started her speech of Session I with general science matter, briefing about various opportunities in science from professional research to entrepreneurship.Dr. L. Akilandeshwari elaborated on the use and application of Argus Lab and Avagadrosoftwares. She explained about application for modeling and visualization of molecules for quantum chemical calculation using Argus Lab. Also she added inputs on constructionofmolecular structures with classical molecular dynamics simulation and structure optimization.

It was described that Avogadro is a software which supports the import of chemical files and generates multiple computational chemistry packages and it is used in many fields of scientific activity such as computational chemistry, molecular modeling bioinformatics and materials science from students to experienced chemists. One of the key demonstrated features for molecule editing. Some chemical groups and structures generated and edited in the workshop includes **Alcohols,** aldehydes, alkanes, alkenes, alkynes, amides, amino acids, carbohydrates, carboxylic acids, etc. In addition to this, structures of DNA and RNA are also demonstrated.

In the session II,Dr. S. AnbuSelvi, Assistant Professor in Chemistry, Sri Sarada College for Women, Salemprovided the ideaand information about state-of-the-art capabilities for electronic structure modelling using Gaussian Software. She explained how to perform semi empirical calculations on some simple atoms and molecules. She also demonstrated the interpretation of IR and NMR data using Gaussian software.

Sample Certificate Issued:



SRI GVG VISALAKSHI COLLEGE FOR WOMEN

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DEPARTMENT OF CHEMISTRY

Certificate of Merit

Ms.Sudarvizhi.N, Student
Nirmala college for women Coimbatore.

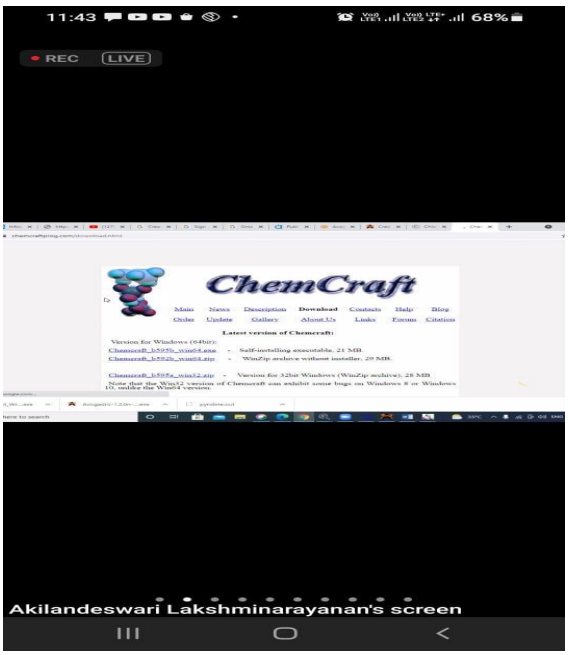
has actively participated in the Two Days National Level Online Workshop on "**Introduction to MOLECULAR MODELLING**" organized by the Department of Chemistry, Sri GVG Visalakshi College for Women, Udumalpet on 18-06-2021 and 19-06-2021.

ORGANIZER
Dr. M. Malarvizhi
Head of the Department,
Chemistry.

PRINCIPAL
Dr. N. Rajeshwari
Sri GVG Visalakshi College
for Women, Udumalpet.

Day 2:

In the Day 2 session, Dr. L. Akilandeshwari introduced different computational software freely available. The usage of Chemcraft, Jmol and Chemsketch was explained. Also the output styles of different softwares and their varied utility in the DFT calculation is well explained. Multiple export formats and their use in other softwares was well elaborated. At the end of the session, she clarified the doubts of the participants in their assignments and working with the Avagadro and Argus Lab software. In the feedback session, participants expressed their gratitude for organizing the workshop which is very much needed and useful. The workshop came to an end with the vote of thanks by Dr.S.Umadevi, Assistant Professor of Chemistry.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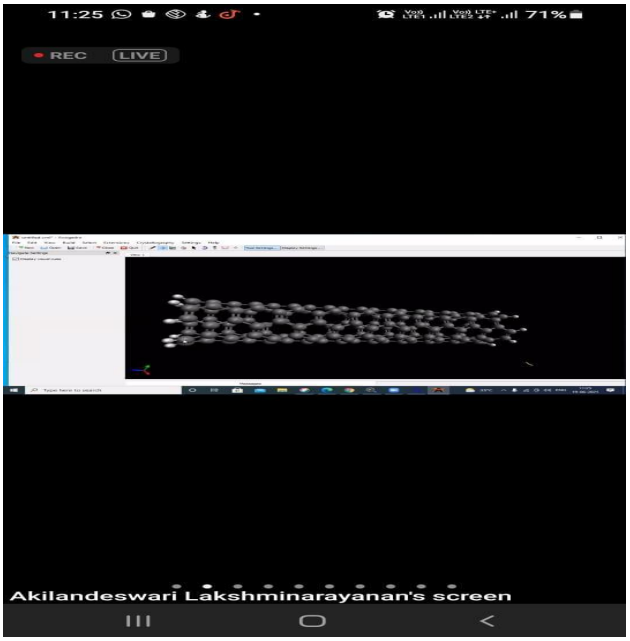
Akilandeswari Lakshminarayanan's screen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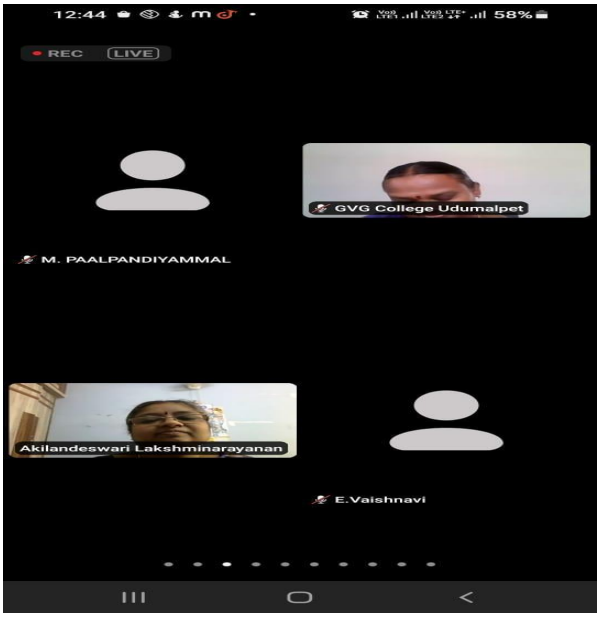
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GVG College Udumalpet
M. PAALPANDIYAMMAL
Akilandeswari Lakshminarayanan
E.Vaishnavi


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