Two Days National Level Work Shop on							
Introduction to Molecular Modelling-Report							
17 th and 18 th 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.

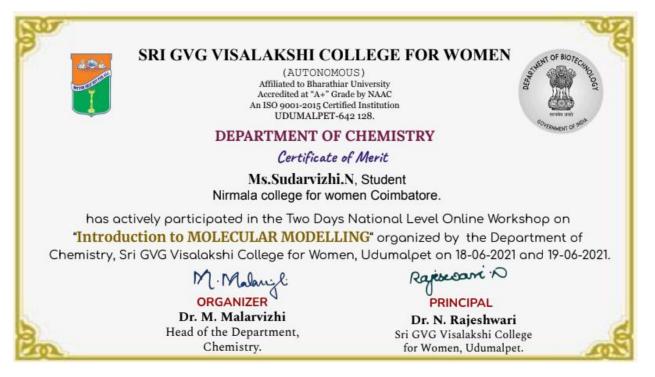
As the first Resource speaker, **Dr. L. Akilandeshwari, Assistant Professor in Chemistry, Sri Sarada College for Women, Salem**was introduced. The resource person started her speech of Session I with general science matter, briefing about various opportunities in science from professional research to 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-ofthe-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.

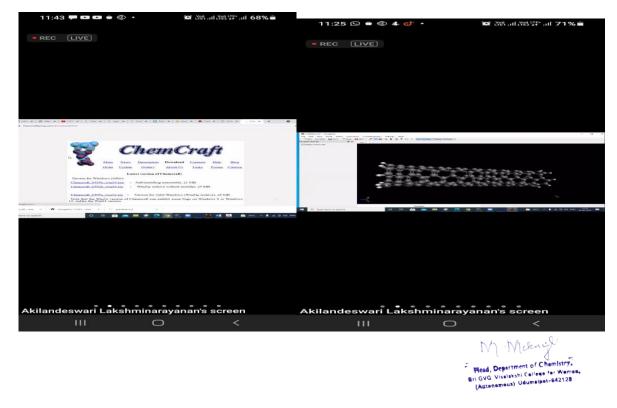
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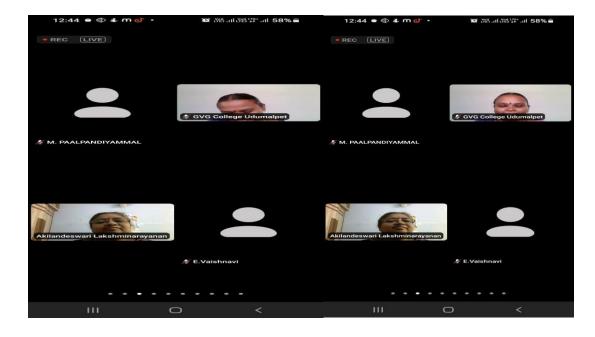
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Day 2:

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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Department of Chemistry

Report on the Workshop "Biochemistry based Experiments" Date : 13.02.2021 Class : II B.Sc. Chemistry, III B.Sc. Chemistry, I B.Sc. Chemistry, I B.Sc. Zoology, II B.Sc. Physics and II B.Sc. Mathematics No. of Beneficiaries : 90

Details of the Resource person: Dr. N. KannikaParameswari M.Sc., M.Phil., PhD Professor Department of BioChemistry, Dr. NGP Arts and Science College Coimbatore

Aim of the workshop

Our aim was to make students become familiar with some biological phenomena and are given the opportunity to acquire some simple skills.

We anticipated students to understand such things as planning and validating: experiments which can be more extensive and perhaps 'open-ended'

These ideas can be extended into the third year of their under graduate programme when students carry out a small research project.

Objectives of the workshop

1. To Illustrate Lectures

- Illustrate phenomena, equipment, by demonstration and personal handling
- Experience handling biological materials Learn standard (or historical) techniques, verify principles
- Realise importance of biochemistry in medicine, industry, etc.

2. To inculcate Laboratory Skills

- to develop manipulative skills
- To learn how to use a particular apparatus
- To learn how to follow a protocol [controls, safety]
- To observe and record accurately
- To process data, (i.e) use statistical methods
- To present data, results, and conclusions

List of Experiments done during the workshop

• Separation of Serum from blood

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- Estimation of alkaline phosphatase in serum
- Estimation of protein in serum by Lowry's method
- Determination of Blood group and Rh type in human
- Determination of the bleeding time of a subject
- Determination of the clotting time of a subject
- Estimation of Haemoglobin in blood
- Isolation, Estimation of chlorophyll and Separation by TLC

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Workshop on First Aid Techniques

17.03.2021

Department of Chemistry organized a workshop on First Aid Techniques on 17.03.2021. The Resource person was the Senior Professor Ms.D.Poongodi from Priya Institute of Paramedical Sciences, Udumalpet. Five Interns from Priya Institute were also present in order to demonstrate some of the first Aid procedures. **60** students from I B.Sc Chemistry and I B.Sc Zoology were the Beneficiaries. The Programme started with the Prayer song followed by the Welcome Address by Dr.M.Malarvizhi, Assistant Professor and Head, Department of Chemistry.

The resource person explained the importance of First aid Techniques and knowing about the performance of First Aid Procedures. She also described the necessity of doing daily Exercise.First and foremost Procedure given due importance in the workshop is CPR. Ms.Poongodi explained the procedure about how to perform a CPR. The intern students demonstrated it clearly. Also the student participants were encouraged to know more about CPR and perform without it any hesitation. Some of the other First Aid techniques explained and demonstrated include Setting a splint, stop the bleeding, treat the burns, help the choking, Fractures and sprains, Nose Bleeding, Bee stings and treat the poison. Each procedure was well explained and demonstrated.

Participants got clarified their doubts. Participants expressed their happiness and gratitude for the useful workshop. The resource person added details about the Ambulance services and their significance at the times of emergency. The programme came to an end with the vote of thanks by Dr.S.Umadevi, Assistant Professor of Chemistry. The Programme was co-ordinated by Dr.M.Malarvizhi, Assistant Professor and Head, Department of Chemistry.



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SRI GVG VISALAKSHI COLLEGE FOR WOMEN

Department of CHEMISTRY in Collaboration with CENTRE FOR ENTREPRENEURSHIP DEVELOPMENT, MADURAI

Organized an Online Workshop on

"Opportunities and Avenues Available for Women Entrepreneurship the Field of Chemistry"

RESOURCE PERSONS

- Dr. R. Jayaraman, Member Secretary, CED TN, Madurai.
- Dr. S. Yaamini Devi, Programme Manager, CED TN Madurai.

DATE -22.05.2021 to 28.05.2021

VENUE -Online Mode (Google Meet)

REGISTRATION LINK-https://forms.gle/cg4Ht7nQB4icKpsu9

WHATSAPP GROUP LINK -

https://chat.whatsapp.com/Ia2IsnoncW6IZjqqldEJ4V

Programme Co-ordinator: Dr.M.Malarvizhi

Assistant Professor and Head Department of Chemistry

Student Co-ordinators : D. Bhavadharani, III B.Sc. Chem M. Paalpandiyammal, II B.Sc.Chem

THEMATICS

□ Entrepreneurial Competencies

□ Entrepreneurial Components

BOG – Avenues available in Chemistry for Women Entrepreneurs
Project Report Preparation & CED TN – Gateway for Women
Entrepreneurs

□ Entrepreneurship Support Institutions & Case study for successful WomenEntrepreneurs

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The Problem of unemployment is becoming a colossal in all of the developing nations. Entrepreneurship is considered one of the most important indicators of societal awareness and rationalization in society's development policies, plans and programs. In order to inculcate a desire to become entrepreneur among the students, *Department of Chemistry in Collaboration with Centre For Entrepreneurship Development, Madurai* Organizes aDBT Star College Scheme Sponsored Online Workshop on"Opportunities and Avenues available for Women Entrepreneurs in the Field of Chemistry " from 22.05.2021 to 28.05.2021. The program is specially designed for the students, who are still pursuing their studies in Colleges and do not have any idea about Entrepreneurship.Purpose of this webinarseries is to create awareness among the students in the essentials of Conceiving, Planning, Initiating and Launching an Economic Activity or an Enterprise Successfullyafter the completion of their studies instead of searching for jobs only. This program is intended to make the participants familiar about the Role and Importance of

- Entrepreneurship
- Process of Setting up of Enterprise
- Preparing Project Reports
- Identifying Marketing Possibilities
- Entrepreneurship Supporting Institutions

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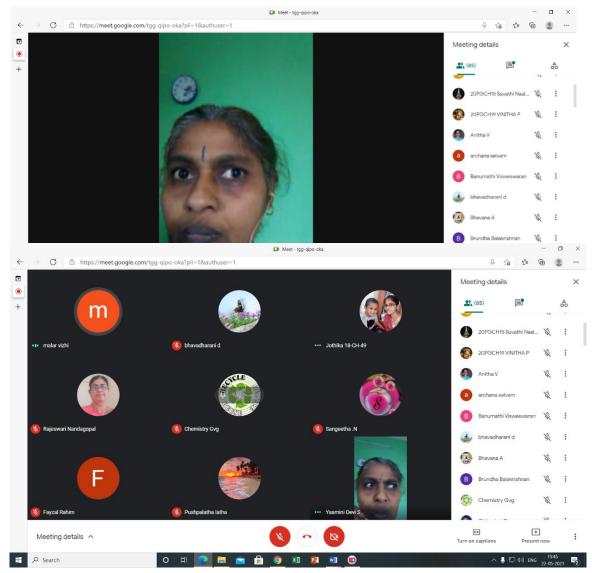
Day 0 Entrepreneurial Orientation

On the First day, the programme was started with the welcome address by Dr.M.Malarvizhi, Assistant Professor and Head, Department of Chemistry, Sri GVG Visalakshi College for Women,Udumalpet. Then, the key note speaker Dr. S. Yamini Devi, Programme Manager,CED TN Madurai, oriented the students about **Entrepreneurship**. She beautifullyexplained the students about requirements of Enterprises.During the session, students were explained about different types of small and medium enterprises around us.Speaker gave overall idea about investment requirements, types of machinery used and other essential requirements in setting up small scale businesses like nail polishing, collection of neem seed, amla&grape leaves, spice grinding & packaging. After her orientation, Dr.N.Rajeswari, Principal, Sri GVG Visalakshi College for Women,Udumalpet delivered her felicitations to the guest speaker. Finally, the programme was ended with the vote of thanks proposed by Dr.S.Umadevi, Assistant Professor,Department of Chemistry, Sri GVG Visalakshi College for Women, Udumalpet.Prototyping to incubation of ideas and materializing them came up for discussion in various sessions during the next day-long programme.

Date: 22.05.2021 Saturday during 3.00- 4.00pm Google Meet Join link - <u>https://meet.google.com/tgg-qipo-oka</u> Attendance Link – <u>https://forms.gle/B4c9uhyuKUWaht4G8</u> Number of Beneficiaries : 88 + 7 **Glimpses:**



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Day 1 Entrepreneurial Competencies

The second day session emphasized the **Entrepreneurial Competencies**such as Opportunity-seeking and Initiative, Persistence, Commitment, Demand for efficiencyand Quality, Taking calculated risks, Goal setting, Information seeking, Systematic planning and monitoring, Independence and Self-confidence etc. and various government schemes supporting entrepreneurship in India were also discussed.

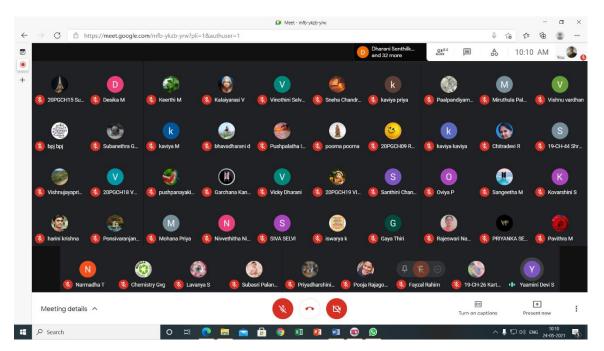
Date: 24.05.2021 N Google Meet Join link - <u>https://meet.google.com/mfb-ykzb-yrw</u>

Monday10.00- 11.00 am

Head, Department of Chemistry, Bri GVG Visalakshi College for Womon, (Autonomous) Udumalpot-642128 Attendance Link – <u>https://forms.gle/Hc3A7acmvAPQWYak9</u> Number of Beneficiaries:120 + 7

Glimpses





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Day 2 Entrepreneurial Components

On the third day, the topics discussed ranged from **Entrepreneurial Components** to **Case Study of Successful Entrepreneur.** The speaker gave wellorganized explanation about the Entrepreneurial Componentssuch as Behavioral Component, Achievement Motivation Training to the Network with Rrganization. Students were motivated by the success story of Lijjat Puppad, the Quin of Herbals (Shenaz hussain) andetc.

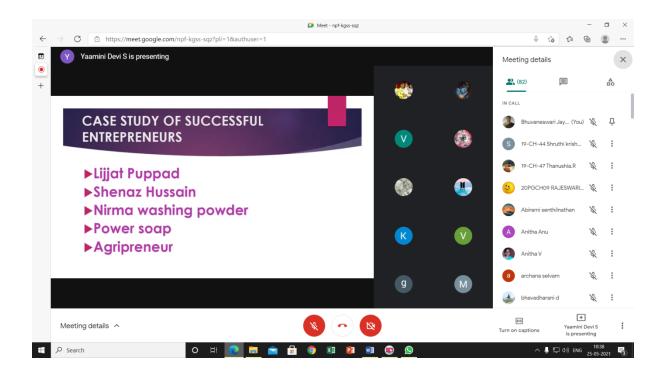
Date: 25.05.2021 Google Meet Join link - <u>https://meet.google.com/npf-kgss-sqz</u> Attendance Link – <u>https://forms.gle/1mHKY4mf5G371Rjs9</u> Number of Beneficiaries : 108 + 7

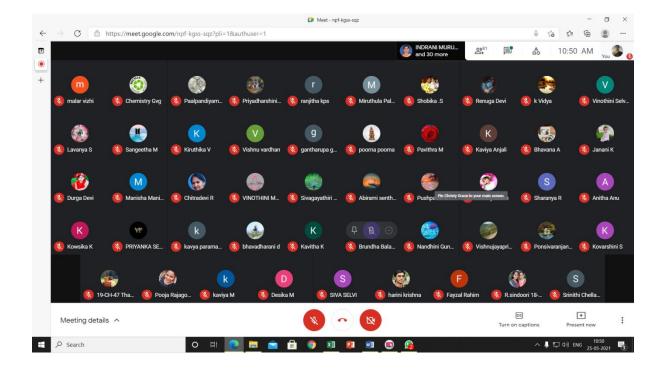
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Monday 10.00- 11.00 am





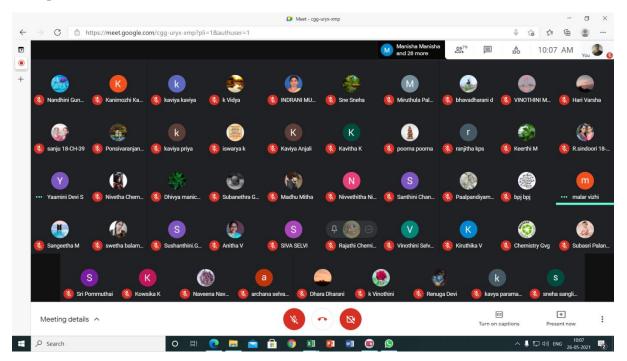
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Day 3 Business Opportunity Guidelines

On the fourth day, students were involved in the self-analysis by doing the Who am I?exercise. After this student were exposed to SWOT(Strengths, Weaknesses, Opportunities, and Threats) analysis. After this analysis, students recognized that SWOT Analysisis a technique for assessing these four aspects of their business.Finally, the speaker well explained the various business opportunities. Students were clear about Identification of business opportunity and Generation of business ideas today.

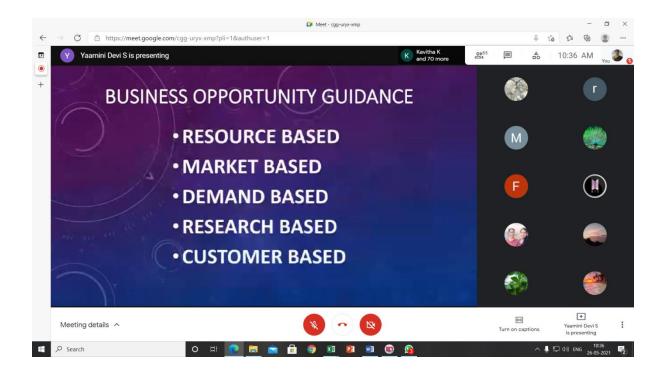
Date: 26.05.2021Monday 10.00- 11.00 amGoogle Meet Join link - https://meet.google.com/cgg-uryx-xmpAttendance Link - https://forms.gle/eT49qkkkmR9WfTni7Number of Beneficiaries : 108 + 7

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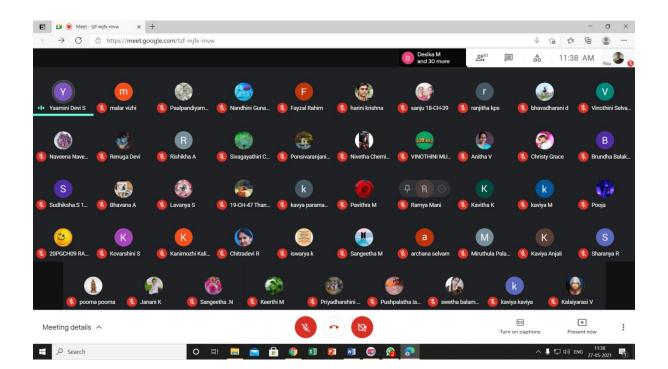
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Day 4 Project Report Writing

The topic of the fifth day is Preparation of a Business Plan. Today's programme was a great learning experience and it provided the students with valuable important tips about the Preparation and Launching the enterprise.

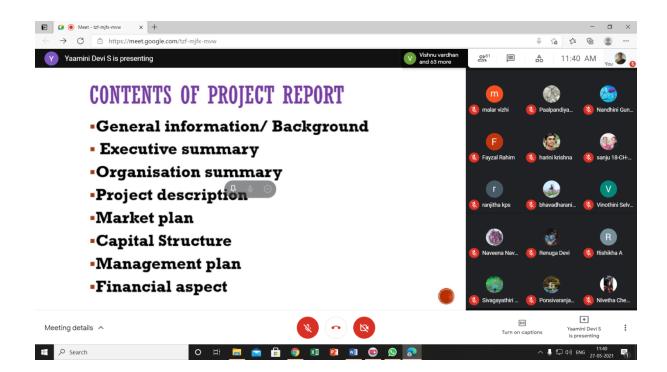
Date: 27.05.2021 Thursday 11.30 am - 12.30 pm Google Meet Join link - <u>https://meet.google.com/tzf-mjfx-mvw</u> Attendance Link – <u>https://forms.gle/BArmYBNJySdqwES89</u> Number of Beneficiaries : 109 + 7

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Day 5 Entrepreneurial Support Institutions

On the last day, **Dr. R. Jayaraman, Member Secretary, CED TN, Madurai,** delivered the talk about Entrepreneurship. His talk was the great motivation to the student community. Later on, the speaker gave overall exposure to the Institutional Support System for Entrepreneurshipwhich has been designed at following four levels: 1. Central Government 2. State Government 3. Non-Government Support System 4. District Industries Centres (DIC). The Following are the few supporting institutions mentioned by the speaker.

- NSIC (National Small Industries Corporation Limited)
- NABARD National Bank for Agriculture and Rural Development
- NI-MSME National Institute for Micro, Small and Medium Enterprises
- SIDO (Small Industries Development Organization)
- SSIB (Small Scale Industries Board)
- SSIDC (Small Scale Industries Development Corporation)
- SISIs (The small industries service institutes)
- DICS (The small industries service institutes)
- MGIRI Mahatma Gandhi Institute for Rural Industrialisation
- Spices and Coir Board
- INDUSTRIAL ESTATES- (Industrial region, industrial park, industrial area, industrial zone, etc.)

Date: 28.05.2021 Thursday 11.30- 12.30 am Google Meet Join link -<u>https://meet.google.com/gni-eeff-rjf</u> Attendance Link – https://forms.gle/XTDnK9AvUjR2H7547 Number of Beneficiaries : 102 + 7

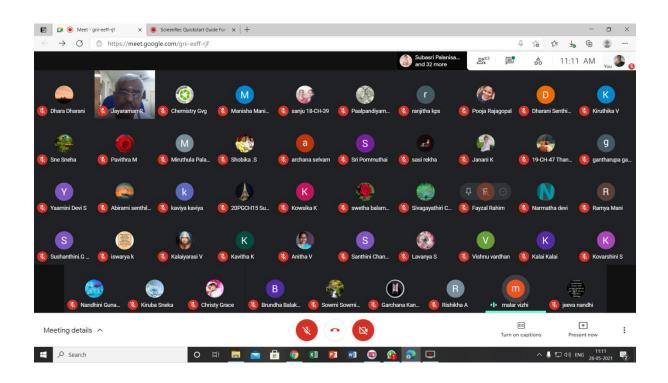
Feedback Link -

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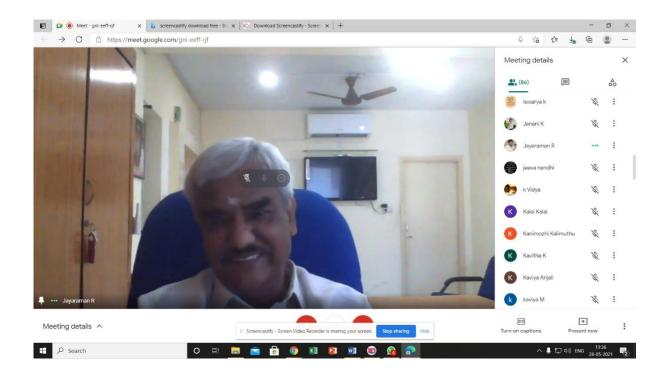
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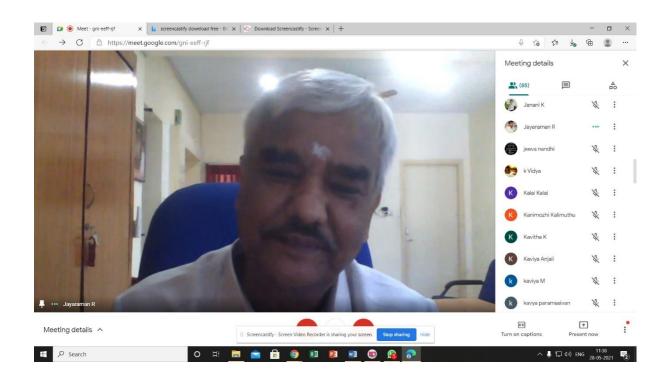
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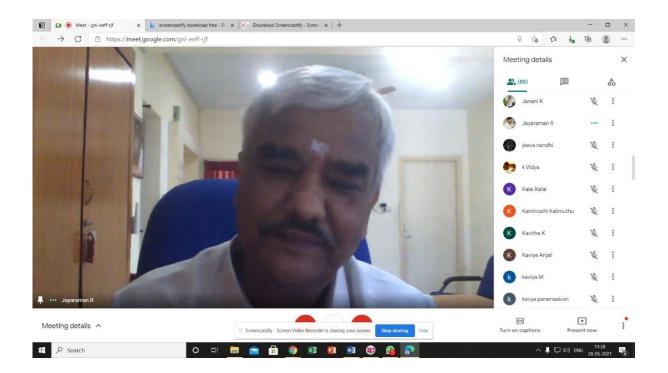
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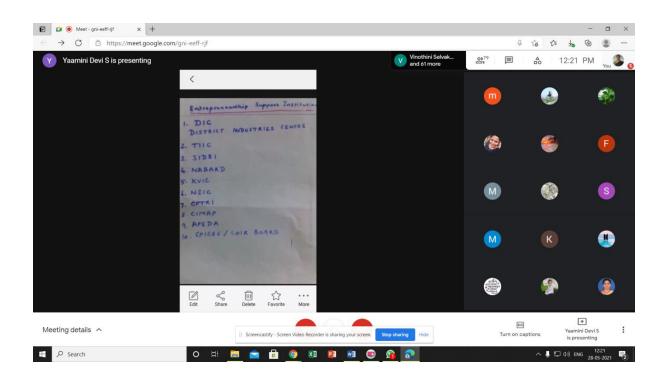
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