



MARUDHAR KESARI JAIN COLLEGE FOR WOMEN, VANIYAMBADI



Recognized u/s 2(f) & 12(B) of UGC Act 1956 - Permanently Affiliated to Thiruvalluvar University

Re-Accredited by NAAC with "A" Grade An ISO 9001:2015 Certified Institution



PG & RESEARCH DEPARTMENT OF PHYSICS ORGANIZED WORKSHOP AN DENSITY FUNCTIONAL THEORY FOR BEGINNERS ON 08.09.2021

INVITATION


**MARUDHAR KESARI JAIN COLLEGE FOR WOMEN, VANIYAMBADI**

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PG & RESEARCH DEPARTMENT OF PHYSICS
Invites you to Workshop on

"Density Functional Theory for Beginners"

RESOURCE PERSONS:




Dr. N. Kanagathara,
Associate Professor,
Department of Physics,
Saveetha School of Engineering,
SIMATS, Chennai.



Dr. R. Usha,
Assistant Professor,
Department of Physics,
Saveetha School of Engineering,
SIMATS, Chennai.

TOPIC: "Density Functional Theory for Beginners" **TOPIC: "Density Functional Theory - A Practical Introduction"**

DATE : 08.09.2021
TIME : 11.00am-01.00pm

LIVE IN 

Registration link: <https://forms.gle/B4kWQZiffXsavmE6>
Admission Link: <https://forms.gle/pavqKyPebP9tgPfd6>
Website: www.mkjc.in

✓ No registration fee
✓ E-Certificate will be provided

Sri. C. Lickmichand Jain
SECRETARY

Dr. M. Inbavalli
PRINCIPAL

Dr. V. Sabari & Dr. C. Pavithra
CONVENORS


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Marudhar Kesari Jain College
for Women
Vaniyambadi - 635 751

AGENDA



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PG & RESEARCH DEPARTMENT OF PHYSICS

Organize

Workshop

on

"Density Functional Theory for Beginners"

Agenda

Date: 08.09.2021

Time: 11.00 am – 12.00 pm

Prayer

Welcome Address


: Ms. P. Praveena,
Assistant Professor,
Department of Physics,
Marudhar Kesari Jain College for Women.

Felicitation Address

: Dr. M. Inbavalli,
Principal,
Marudhar Kesari Jain College for Women.

Chief Guest Introduction - I

: Ms. A. Reena Arul Vani,
Assistant Professor,
Department of Physics,
Marudhar Kesari Jain College for Women.


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Address By Chief Guest	: Dr. N. Kanagathara, Associate Professor, Department of Physics, Saveetha School of Engineering, SIMATS, Chennai.
Chief Guest Introduction - II	: Ms. M. Anchana, Assistant Professor, Department of Physics, Marudhar Kesari Jain College for Women.
Address By Chief Guest	: Dr. R.Usha, Assistant Professor, Department of Physics, Saveetha School of Engineering, SIMATS, Chennai.
Vote of Thanks	: Ms.B.Prabavathi, Assistant Professor, Department of Physics, Marudhar Kesari Jain College for Women.
National Anthem	


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PG & RESEARCH DEPARTMENT OF PHYSICS ORGANIZED WORKSHOP AN DENSITY FUNCTIONAL THEORY FOR BEGINNERS ON 08.09.2021

REPORT

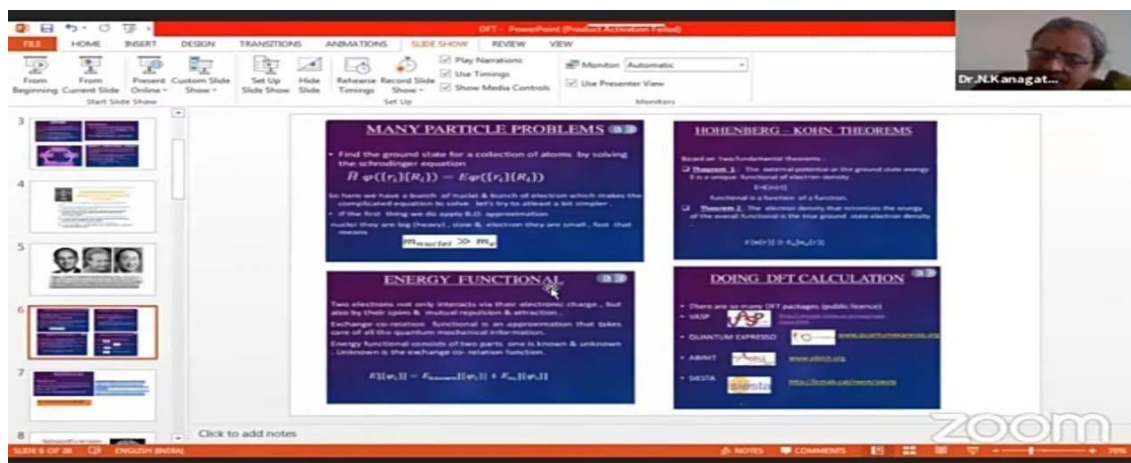
PG & Research Department of Physics organized a workshop in title "Density Functional Theory for Beginners" on 08.09.2021. The Program started with invocation of Prayer followed by welcome address delivered by Ms. P. Praveena, Assistant Professor, Department of Physics, MKJC. The Chief Guest introduction was given by Ms. A. Reena Arul Vani, Assistant Professor, Department of Physics, MKJC. Next the session was handover to the resource person Dr. N. Kanagathara, Associate Professor, Department of Physics, Saveetha School of Engineering, SIMATS, Chennai. She spoke about "Density Functional Theory for Beginners" and from her speech students learned the fundamentals in DFT. Later the session was taken over by Dr. R. Usha, Assistant Professor, Department of Physics, Saveetha School of Engineering, SIMATS, and Chennai. She gave a talk on "Density Functional Theory-A Practical Introduction" which was very useful for determining the properties of the crystals theoretically. Totally 179 members were participated.

A Verbal gratitude was delivered by Ms. B. Prabavathi, Assistant Professor, Department of Physics, MKJC. The Program concluded with the National Anthem.

Head of the Department

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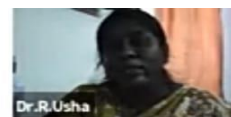
PHOTO



Introduction

- The most important orbitals in molecules for reactivity are the two so called **frontier orbitals**.
- These are called the **HOMO** and **LUMO**

	LUMO lowest unoccupied molecular orbital	<ul style="list-style-type: none"> LUMO receives electrons lowest energy orbital available characteristic for electrophilic component
	HOMO highest occupied molecular orbital	<ul style="list-style-type: none"> electrons from the HOMO are donated most available for bonding most weakly held electrons characteristic for nucleophilic component



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