

# GOVERNMENT COLLEGE FOR WOMEN (AUTONOMOUS)

KUMBAKONAM – 612 001

Affiliated to Bharathidasan University

DST - CURIE Sponsored Institution

IV Cycle of Accreditation



☎ 0435 – 2401391

✉ principal@gcwk.ac.in



## NATIONAL LEVEL WORKSHOP ON " MATERIALS MODELLING USING QUANTUM ESPRESSO THEORY AND PRACTICE FOR BEGINNERS"

**DATE** : 29-07-2019, 30-07-2019

**SPEAKER** : Dr.C.S.Praveen,  
Dr.K.C.Bhamu,  
Dr.Subramanyam Sapatti.

<p><b>VALEDICTION</b> 4.00 pm - 4.30 pm</p> <p><b>Valedictory Address:</b> <b>Dr.G.VIRUTHAGIRI</b> Assistant Professor of Physics Govt. College for Women (A) Kumbakonam-612 001.</p> <p><b>Distribution of Certificates :</b> <b>Dr. P. CYNTHIA SELVI</b> Principal Govt. College for Women (A) Kumbakonam-612 001</p> <p>National Anthem.</p> <p><i>Thank you.....</i></p>	<p><b>UGC SPONSORED NATIONAL LEVEL WORKSHOP ON</b></p> <p><b>"MATERIALS MODELLING USING QUANTUM ESPRESSO - THEORY AND PRACTICE FOR BEGINNERS" (QE19)</b></p> <p>Venue : SSS Seminar Hall Date : 29<sup>th</sup> &amp; 30<sup>th</sup> July - 2019 Time : 10.00 AM</p>  <p><b>Organized by</b></p> <p><b>PG &amp; RESEARCH DEPARTMENT OF PHYSICS</b> <b>GOVERNMENT COLLEGE FOR WOMEN (AUTONOMOUS)</b> KUMBAKONAM – 612 001. <a href="http://www.gcwk.ac.in">www.gcwk.ac.in</a></p> <p><i>All are Cordially Invited</i></p>
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## INAUGURATION


- 10.00 am: Invocation
- 10.05 am: Welcome Address – Dr. R. RADHA  
Convener  
Associate Professor & Head  
Department of Physics  
Govt. College for Women (A)  
Kumbakonam-612 001
- 10.15 am: Presidential Address – Dr. P. CYNTHIA SELVI  
Principal  
Govt. College for Women (A)  
Kumbakonam-612 001
- 10.25 am: Felicitations – Dr. S. AHILA  
Associate Professor & Head  
Department of Tamil  
Govt. College for Women (A)  
Kumbakonam-612 001
- Dr. S. VENKATALAKSHMI  
Controller of Examinations  
Govt. College for Women(A)  
Kumbakonam-612 001
- 10.30 am: Vote of Thanks – Dr. T. THILAGAVATHI  
Organizing Secretary  
Assistant Professor of Physics  
Govt. College for Women (A)  
Kumbakonam-612 001
- 10.30 am -10.45 am Tea Break

## PROGRAMME

Date : 29.07.2019

TIME	SESSION
10.00 am – 10.30 am	Inauguration
10.45 am – 11.30 am	Introduction to Density Functional Theory Calculations (Dr. Praveen C. S.)
11.30 am – 12.15 pm	Applications of Density Functional Theory (Dr. K. C. Bhamu)
12.15 pm – 01.00 pm	Basic Linux for Computation (Dr. Subramanyam Sapatti)
01.00 pm – 02.00 pm	Lunch
02.00 pm – 03.15 pm	Quantum Espresso input description (Dr. C. S. Praveen, Dr. K. C. Bhamu, Dr. Subramanyam Sapatti) (Hands-On)
03.15 pm – 03.30 pm	Tea Break
03.30 pm – 04.30 pm	Quantum Espresso input description (Dr. C. S. Praveen, Dr. K. C. Bhamu, Dr. Subramanyam Sapatti) (Hands-On)
<b>Date : 30.07.2019</b>	
09.45 am – 10.45 am	Geometry Optimization (Dr. C. S. Praveen) (Hands-On)
10.45 am – 11.00 am	Tea Break
11.00 am – 12.00 pm	Simple Calculations using Quantum Espresso (Hands On) (Dr. K. C. Bhamu)
12.00 pm – 01.00 pm	Visualisation using XCrySDen (Dr. C. S. Praveen) (Hands On)
01.00 pm – 02.00 pm	Lunch
02.00 pm – 03.00 pm	Post-processing using Quantum Espresso (Dr. C. S. Praveen, Dr. K. C. Bhamu, Dr. Subramanyam Sapatti) (Hands-On)
03.00 pm – 03.15 pm	Tea Break
03.15 pm – 04.00 pm	Post-processing using Quantum Espresso (Hands-On) (Dr. C. S. Praveen, Dr. K. C. Bhamu, Dr. Subramanyam Sapatti)



  
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*S. Arul*  
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