



# St. Xavier's College For Women, Aluva

( Affiliated to Mahatma Gandhi University, Kottayam & Re-accredited by NAAC with A Grade )

## UGC SPONSORED NATIONAL WORKSHOP ON COMPUTATIONAL CHEMISTRY AND ITS APPLICATIONS

29<sup>th</sup> & 30<sup>th</sup> September 2014


Organised by Department of Chemistry


In collaboration with Post Graduate and Research Department of Chemistry,  
Sacred Heart College, Thevara

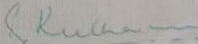
### Certificate

This is to certify that Dr. ABI.T.G, Assistant Professor ~~has participated/presented a~~  
~~paper entitled~~ Dept. of Chemistry, Sacred Heart college, Thevara / served as a resource person  
in the National Workshop on Computational Chemistry and its Applications held on 29<sup>th</sup> & 30<sup>th</sup> September 2014.



  
**Ms. Shenya Festus**  
Co ordinator

  
**Ms. Beena Varghese**  
Convener

  
**Sr. Reethamma V.A.**  
Principal



ST XAVIER'S COLLEGE FOR WOMEN  
ALUVA, KERALA

DEPARTMENT OF CHEMISTRY

**NATIONAL WORKSHOP  
ON  
COMPUTATIONAL  
CHEMISTRY AND  
ITS APPLICATIONS**

29th & 30th September, 2014 Venue: College Seminar Hall

Sponsored by  
**UNIVERSITY GRANTS COMMISSION**  
New Delhi

In collaboration with Post graduate and  
Research Department of Chemistry, S.H. College, Thevara

## Programme

### 29th September 2014

08.30 am - 09.00 am : Registration  
09.00 am - 09.30 am : Inaugural session

### Technical session I 09.30 am - 11.15 am

#### Using Computational Chemistry to Predict and Understand Molecular Properties

Dr. Bhanu Prakash Kotamarthi, Chief Scientist, Inorganic and Physical Chemistry Division,  
Indian Institute of Chemical Technology, Hyderabad.

11.15 am - 11.30 am : Tea Break

### Technical session II 11.30 am - 01.00 pm

#### Introduction to Computational Chemistry

Dr. Cyriac Mathew, Associate Professor  
Former Vice Principal and Head of Department  
Department of Chemistry, St. Albert's College, Ernakulam.

01.00 pm - 01.30 pm : Lunch

### Technical session III 01.30 pm - 03.30 pm

#### Chemistry with Computers - What and How?

Dr. Parameswaran Pattiyil, Assistant Professor, Department of Chemistry,  
National Institute of Technology, Calicut.

03.30 pm - 03.45 pm : Tea Break

03.45 pm - 05.00 pm : Paper Presentations

### 30th September 2014

### Technical session IV 09.00 am - 10.30 am

#### Modelling of Chemical Reactions Using QM/MM and MD Simulations

Dr. Abi T. G., Assistant Professor, Department of Chemistry,  
Sacred Heart College, Thevara, Kochi.

10.30 am - 10.45 am : Tea Break