

Workshop on
Computational Portal in
Chemistry

Organised jointly by

**Kerala Education Grid [KEG]
&
Indian Institute of Technology, Madras**

Dates: March 18-19, 2005

Venue & Contact Detail

Education Grid Resource Centre,
IIITM-K Project Wing, GF, Nila,
Technopark, Thiruvananthapuram- 695 581
Tel: 0471-2700965; 3093500 Fax: +91-471-2527568
E-mail: kegworkshop@iiitmk.ac.in
Home: <http://www.edugrid.ac.in/>

ABOUT THE ORGANISERS

This workshop is being organized jointly by the Kerala Education Grid Resource Centre at Indian Institute of Information Technology & Management-Kerala (IIITM-K) and the Department of Chemistry, Indian Institute of Technology – Madras.

Kerala Education Grid [KEG] is an initiative undertaken by the Govt. of Kerala to enhance the quality education to all students of higher education in the State. As part of this project several activities are being undertaken to build web-resources, enhance quality of teaching and exposing the teachers to technology enhanced learning and teaching environment. For more information, please visit: <http://www.edugrid.ac.in>

The Dept. of Chemistry at IIT-Madras has been a leading research school in Computational Chemistry. Following their discussions with the KEG, a trial version of the Computational Chemistry Portal has been started in IIT Madras. We propose to deploy the same for the benefit of researchers and scholars interested in Computational Chemistry.

WORKSHOP AT A GLANCE

All traditional branches of Chemistry such as Organic, Inorganic, Physical, Biochemical and Pharmaceutical are now increasingly using computational methods in research and teaching. Problems such as molecular structure, electric and magnetic properties of materials, molecular spectroscopy, reaction dynamics, protein-protein interactions, drug design etc. are all within the reach of the general chemist with no extensive computational or theoretical skills. Computational chemistry has thus become a laboratory tool. This workshop aims at a group of college/university teachers and research scholars interested in using computational chemistry tools in their teaching/research.

The programme consists of:

- (a) Introductory lectures on the methods of computational chemistry
- (b) Hands-on training of participants in the use of public-domain software
- (c) Training on the use of the Computational Chemistry Portal using web browsers
- (d) Proposal for periodic updating of the portal with software of interest to the Chemistry teaching community

SCHEDULE

Day-1: 18 March 2005

Sess No.	Topic	Faculty	Time (hrs.)
1	Introduction to Computational Chemistry	Prof. M S Gopinathan	9.00-10.00
Tea Break			
2	Introduction to Grid Portal architecture and web usage of packages	Dr M S Krishnan	10.15-11.15
3	Introduction to Grid Portal architecture and web usage of packages	Dr Sanjay Kumar	11.15-12.15
4	Discussions		12.15-13.00
Lunch Break			
5	Tensor Contraction Engine	Dr. Venkatesh Choppella	14.00-14.45
5	Practical Session	(a) Accessing Portals and Packages (b) Using "Gamess" ab initio Package	15.00 –17.30 15 minutes tea break at 14.45 hrs.

Day-2: 19 March 2005

Sess No.	Topic	Faculty	Time
1	Introduction to Molecular Mechanics & Molecular Dynamics	Prof. M S Gopinathan	9.00-10.00.
Tea Break			
2	Introduction to visual aided chemical concepts and computation	Dr M S Krishnan	10.15-11.15
3	Density functional theory and its application in chemistry	Dr Sanjay Kumar	11.15-12.15
4	Discussions		12.15-13.00
Lunch Break			
5	Practical Session	(a) Using "Tinker" MM and MD Packages (b) DFT calculations using Gamess and other packages	14.00 –17.00 15 minutes tea break at 15.30
6	Feedback Session		17.00-18.00

COURSE FACULTY

Prof. M S Gopinathan- Professor of Chemistry, IIT-Madras. He has done pioneering work in various areas in chemistry, such as experimental and theoretical magnetic resonance, atomic and molecular quantum chemistry and nonlinear dynamics. Recently he has turned his attention to experimental and modeling studies on nonlinear phenomena in chemistry, biochemistry and physiology. He is a Fellow of INSA. Home: <http://chem.iitm.ac.in/msgopinathan.htm>

Dr. Mangala Sunder Krishnan- Associate Professor of Chemistry, IIT-Madras and the Coordinator for the National Programme on Technology Enhanced Learning funded by the MHRD, Government of India. His research interests are in analysis of coupled energy states and molecular properties such as dipole moment and polarizabilities and understanding experimental high resolution spectra of weak molecular complexes and considerably non-rigid molecules.

Home: <http://chem.iitm.ac.in/kmangalasunder/kmsresume.htm>

Dr Sanjay Kumar- Assistant Professor of Chemistry, IIT Madras. His research area is theoretical molecular reaction dynamics. His research group is engaged in high-level *ab initio* quantum mechanical calculations and quantum dynamics to predict the rates of elementary chemical reactions. His current research involves non-adiabatic collisions, quantal characterization of metastable negative ions and their fragmentation pathways.

Dr Venkatesh Choppella- Associate Professor at IIITM-K. He works in the area of compilers, programming languages, domain-specific languages for scientific computation, software engineering, automated deduction, and verification. Earlier he had worked on the Tensor Contraction Engine at Oak Ridge National Labs, USA. This involved developing a domain-specific language that allows chemists to specify the computation in a high-level Mathematica-style language. Home: <http://www.iiitm.ac.in/~choppell>

Registration form. The maximum **number of seats will be limited to 25** and will be filled in first come first serve basis. Five seats will be reserved for participants from the industry. Participation fee for members from academic & research institutions would be sponsored by the KEG project. The registration fee for participants from industries and commercial organizations is Rs. 5000/- per participant. The fee is to be paid in the form of DD in favour of Director, IIITM-K, payable at Thiruvananthapuram

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Registration Form

Name(s) of participants

(1).....

e-mail:.....Phone:.....

Reason why this workshop is of interest to you:

(2).....

e-mail:.....Phone:.....

Reason why this workshop is of interest to you:

Name of Organization and Address:

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.....
.....

Phone:

Fax:

e-mail:

Send filled up registration form to:



Director,

Indian Institute of Information Technology & Management-
Kerala Project Wing, Ground Floor, Nila
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