

Annual Report 2012-2013

Centre for Modelling Simulation and Design (CMSD)

PREAMBLE

The study of passage from the micro world of atoms and molecules to the macro world of solids, liquid and gases calls for an understanding of a variety of phenomena in physics, chemistry, biology and engineering science and technology and related areas. Atomic lasers, molecular computers, drug-receptor interactions, industrial catalysts, lubricants, and industrially important materials form part of this continuum and an understanding of this evolution needs all the three components of research, viz. theory, experiment and computation. Computer-based simulations now form an integral part of modern research methodology and in this era of science-driven-engineering and directed basic research, the role of scientific research, based on modeling, simulation and design, is of paramount importance. The primary requisite in using the third avenue of research for solving complex problems is a working, state-of-the-art High Performance Computing (HPC) center.

The University of Hyderabad, having expertise in many of the above areas, fully appreciates the inter-dependence of Science, Engineering and Technology, and launched a uniquely conceived new programme. This initiative was launched through an imaginative programme of the UGC (recognizing the University for its potential for excellence) by establishing a designated Centre for such activity (Centre for Modelling Simulation and Design – CMSD). This programme has been receiving generous support from DST under its FIST program.

CMSD aims to nurture cross-disciplinary bridges, which are effective in generating new knowledge and creative explorations. The human resources generated from such efforts will be invaluable. Training individuals and organizations in specific hardware and software, undertaking of consultancy and turnkey projects, help convert real life phenomena into appropriate mathematical and computational models etc., are some of the important tasks that CMSD has embarked on. This centre became operational from its new premises in December 2004.

One of the unique academic features of this centre is that all the active computational scientists working in widely different academic disciplines in the university campus are associate faculty of the CMSD, and contribute their expertise and experience in furthering its objectives. Some of the research interests of these members include: physics of low dimensional systems, topological defects in fluids in restricted geometries, critical phenomena in complex fluids and magnetic systems, Monte Carlo simulations and development of novel sampling techniques, genomics and bioinformatics, protein folding, cognitive neuroscience, computational intelligence, natural language understanding, Very Large Scale Integration (VLSI), quantum

chemistry and Density Functional Theory(DFT), molecular modeling, drug design and delivery, design of new materials etc

Currently, CMSD has a 25.0 Teraflop Facility which is fully networked and consists of the following hardware:

COMPUTATIONAL FACILITY

- 6 SMP Systems with total of 192 CPUs [1 x IBM p690 (32 Power 4), 3 x IBM p690 (96 Power 4+), 1 x IBM p595 (64 Power 5)], 1 x IBM p595 (64 Power 5+) @ 2.3 GHz, 512 GBytes of main memory and 4 TBytes of storage.
- A CDAC PARAM SUN cluster consisting of 16 nodes (each with dual xeon processors) and 32 GB memory.
- High end workstations such as 6 x SGI Octone 2, 2 x SUN Blade 2000, 6 x IBM Intellistations etc.
- SGI Altix 4700 a 128 core (Dual Core, Itanium2 9150M 1.67 GHz) shared memory architecture based Unix server comprising of 512 GB RAM
- SGI Altix ICE 8200 EX Cluster [Enhanced] with 1024 core high performance, high throughput and high availability cluster comprising of 1 GB/core memory, built using Infiniband Interconnect.
- SGI XE1300, 2 x Quad core @ 3.0GHz, 4 GB RAM, 146 GB HDDA 128 core Windows CCS/HPC Cluster.
- SGI IS4600 x 2, 100 TBytes of shared Storage system (FC, SATA) for delivering very demanding data intensive environment, leading to High Performance & Productive Computing Facility, through SGI Altix 450 x 2, 8 core, 48 GB RAM, Montvale 1.67 MHz storage servers.
- SGI Spectra T120 Library, 2 x LTO Gen-4 Drives scalable to 6, Spectralogic 100 slots and 60 units of Media, a good tape backup system to archive data with time stamping.
- Management Servers: SGI Altix 250 SERVER x9 (2U), 2 x Quad core, E5472, 3.00 GHz, 1600 FSB, 12MB Cache, 8GB RAM, 6 x 145GB SAS HDD/15K
- Parallel file system to allow bulk I/O operations.
- IBM POWER 7 - 755 Server with - 4 x 8 core 3.3 GHz Power 7 Processor, 2 x 146 GB DASD, 128 GB DDR3 RAM,
- IBM StoreWize V7000 based Storage with 60TB RAW Storage Capacity (30 x 2 TB Disks)

To support various application domain areas the following software are deployed on the above hardware: Accelrys Suite, Gaussian 2003, MOPAC, Relibase+,

Molpro, ADF, GCG Wisconsin, SPSS, Mathematica, Statistica, GAMS, RATS, Matlab with toolboxes, CFX 5.7, 3D Studio Max, iSIGHT Pro, BOS, BEAMPRO, GAMESS, SPARTAN 2003, NAG Fortran SMP Library, Empire 3D V4.2, Ansys Multiphysics, AWR (Microwave Office), Full Wave Sonnet, ArcGIS, ArcMIS, Cadence, ISATIS, TURBOMOL, Image Processing S/W like ERDUS, etc.

VISUALIZATION FACILITY

- NVIDIA Quadro FX 5600 Active Stereo Graphics Card
 - Windows XP Professional
 - 750GB SATA Disk Drives
 - 22" LCD Monitor
- SGI Image generator – VN200 system,
 - DVD Drive, 2xGbE Ethernet,
 - Two quad-core Intel Xeon E5462 2.8GHz processors
 - 16GB DDR2 800 REG ECC Memory
 - NVIDIA Quadro FX 5600 Active Stereo Graphics Card
 - SLES10 Linux
 - 160GB SATA Disk Drives
 - 22" LCD Monitor
- Christie Mirage HD6 3chip stereo DLP projector and Lens
- Screen – 9ft x 6ft fabric
- Crosspoint 450 Plus 84HVA Matrix Switcher RGB for Video & Stereo Audio
- Video and Audio interface – Extron RGB109
- Audio Amplifier
- NuVision Active Stereo Glasses
- NuVision Stereo Emitters (mid range)
- Wireless AMX control system
- CEI Ensign Application Software
- Remote Visualization Software Single User

Adjunct Professor

1. Prof. Anil Kumar, Dept. of Physics & NMR Research Centre,
Indian Institute of Science (June 20, 2009 to June 19, 2012)

Visiting Professor

1. Dr. M R Reddy, Metabasis Therapeutics, San Diego, USA.
2. Dr. Ingua Ramarao, Computational Physicist, East West
Enterprises Inc., USA

Post-Doctoral Fellows

Dr (Ms) G. Sai Preeti, recipient of UGC Dr. D. S. Kothari Postdoctoral Fellowship has joined CMSD on February 2011, for a period of 3 years. She previously worked as a Post doctoral research

assistant in the Department of Chimica Fisica ed Inorganica, Università di Bologna, funded by the European Council project 'BIND' after obtaining her PhD from University of Hyderabad.

Dr. Jayasri, has been continuing in CMSD as a post-doctoral fellow supported by PURSE.

Papers Published

Dr. G. S. Vaitheeswaran, Assistant Professor, ACRHEM.

1. K. Ramesh Babu, **G. Vaitheeswaran**, 2013, “Structural, elastic and thermodynamic properties of KN_3 and RbN_3 : A van der Waals density functional study” **Solid State Sciences**, In press (IF: 1.89)
1. J. Ramanna, N. Yedukondalu, K. Ramesh Babu, **G. Vaitheeswaran**, 2013, “Ab initio study of electronic structure, elastic and optical properties of anti-perovskite type alkali metaloxyhalides” **Solid State Sciences**, 120.
2. S. Appalakondaiah, **G. Vaitheeswaran**, S. Lebègue, 2013, “A DFT study of structural, elastic, vibrational and quasi particle band structure of solid nitro methane” **Journal of Chemical Physics**, 138, 184705. (IF: 3.3)
4. N. Yedukondalu, Vikas D Ghule and **G. Vaitheeswaran**, 2013, “Pressure induced structural phase transition in solid oxidizer KClO_3 : Ab initio study” **Journal of Chemical Physics**, 138, 174701. (IF: 3.3)
5. S. Appalakondaiah and **G. Vaitheeswaran**, 2013, “Structural properties of solid nitromethane: A Density functional study” **AIP Conference Proceedings**, 1512, 830.
6. **G. Vaitheeswaran** and K Ramesh Babu, 2012, “Metal azides under pressure: an emerging class of high energy density materials”, **J. Chemical Sciences**. 124, 1391. (IF: 1.17)
7. N. Yedukondalu, Vikas D Ghule and **G. Vaitheeswaran**, 2012, “Computational study of structural, electronic and optical properties of crystalline NH_4N_3 ” **J. Phys. Chem. C**. 116, 16910. (IF: 4.8)
8. S. Appalakondaiah, **G. Vaitheeswaran**, S. Lebegue, N. E. Christensen, A. Svane, 2012, “Effect of vanderWaals interactions on structural and elastic properties of black phosphorus” **Phys. Rev. B**, 86, 035105. (IF: 3.691)
9. K. Ramesh Babu, **G. Vaitheeswaran**, 2012, “Ab initio study of structural and vibrational properties of KN_3 under pressure” **Chem. Phys. Lett.** 533, 35. (IF: 2.337)
10. Ch. Bheema Lingam, K. Ramesh Babu, Surya P Tewari and **G. Vaitheeswaran**,

2012, “Density functional study of Electronic, Bonding, and Vibrational Properties of $\text{Ca}(\text{NH}_2\text{BH}_3)_2$ ” **J. Comp. Chem.** 33, 987. (IF: 4.05)

11. Ch. Bheema Lingam, K. Ramesh Babu, Surya P Tewari and **G. Vaitheeswaran**, 2012, “High pressure study of structural and vibrational properties of ammonia borane” **J. Phys. Conf. Series** 377, 012088
12. N. Yedukondalu, **G. Vaitheeswaran**, 2012, “Vibrational properties of BaClF , BaBrF and BaIF under pressure” **J. Phys. Conf. Series**, 377, 012070.
13. Ch. Bheema Lingam, K. Ramesh Babu, Surya P Tewari and **G. Vaitheeswaran**, 2011, “Electronic structure and optical properties of $\text{Ca}(\text{NH}_2\text{BH}_3)_2$ studied from GW calculations” **J. Phys Chem C**, 115, 18795. (IF: 4.8)
14. N. Yedu kondalu, K. Ramesh Babu, Ch. Bheema Lingam, D.J. Singh, **G. Vaitheeswaran**, V. Kanchana, 2011, “Electronic structure, optical and bonding properties of alkaline-earth halofluoride scintillators BaClF , BaBrF , BaIF ”, **Phys. Rev. B**, 83, 165117 (IF: 3.691)
15. Ch. Bheema Lingam, K. Ramesh Babu, Surya P Tewari, **G. Vaitheeswaran**, 2011, Structural, electronic, bonding and elastic properties of NH_3BH_3 : A Density functional study, **J. Comp. Chem**, 32, 1734. (IF: 4.05)
16. K. Ramesh Babu, Ch. Bheema Lingam, Surya P Tewari, **G. Vaitheeswaran**, 2011, High-pressure study on Lithium azide from density functional calculations, **J. Phys. Chem A**, 115, 4521. (IF: 2.946)
17. **A. Waśkowska**, **L. Gerward**, **J. Staun Olsen**, **K. Ramesh Babu**, **G. Vaitheeswaran**, **V. Kanchana**, **A. Svane**, **V.B. Filipov**, **G. Levchenko** and **A. Lyaschenko**, 2011, “Thermo-elastic properties of ScB_2 , TiB_2 , YB_4 and HoB_4 : Experimental and Theoretical studies”, **Acta Materialia**, 59, 4886-4894 (IF: 3.781)
18. K. Ramesh Babu, Ch. Bheema Lingam, S. Auluck, Surya P Tewari, **G. Vaitheeswaran**, 2011, Structural, thermodynamic and optical properties of MgF_2 studied from first principles theory, **J. Solid State Chem** 184, 343. (IF: 2.159)
19. Ch. Bheema Lingam, K. Ramesh Babu, Surya P Tewari, **G. Vaitheeswaran**, 2011, Quantum chemical studies on BeH_2 oligomers, **Computational and Theoretical Chem** 963, 371. (IF: 1.228)

20. Ch. Bheema Lingam, K. Ramesh Babu, Surya P Tewari, **G. Vaitheeswaran** and S. Lebègue, 2011, Quasi particle band structure and optical properties of NH_3BH_3 **Phys. Status Solid RRL** **5**, No:1, 10. (IF: 2.815)

Prof. James Raju :

1. Best paper award given to my student Mr.S.Bashaiah for the paper titled, "**Fabrication of high dielectric constant and low loss X band ceramic waveguide window for high power microwave applications**". **S.Bashaiah, Pramod K Sharma and K.C.James Raju** at CODEC 2012, the 5th International conference on Computers and Devices for Communication, held during December 17-19, 2012 at Institute of Radio Physics and Electronics, Kolkota.
2. "Design of Ultra wideband Bandpass filter in Low Temperature Cofired Ceramic (LTCC) Technology", Pavan, C.L.N.; **K.C.James Raju**, presented at IEEE Prime Asia 2012 held during Dec 5-7, 2012 at BITS, Hyderabad, India.
3. "Fabrication of High Dielectric Constant and Low Loss X Band Ceramic Waveguide Window for High Power Applications." S.Bashaiah, Pramod K.Sharma and **K.C.James Raju** presented at "5th International conference on Computers and Devices for Communication", held during 17-19, December, 2012 at Institute of Radio Electronics, Kolkota.
4. "Vertical interconnect modeling between GCPWs in LTCC technology," Pavan, Ch.L.N.; **K.C.James Raju**; presented at 2012 Asia Pacific Conference on Postgraduate Research in Microelectronics and Electronics (PrimeAsia),held during 5-7, December 2012 at BITS, Hyderabad.
5. "Design of resonator based ultra wideband bandpass filter in Low Temperature Cofired Ceramic Technology", Ch L N Pavan, **K.C.James Raju**, presented at "5th International conference on Computers and Devices for Communication", held during 17-19, December, 2012 at Institute of Radio Electronics, Kolkota.
6. "Microwave Resonators with High K Dielectrics and Ferroelectrics", **K.C.James Raju**, Invited talk at 17th National Seminar on Ferroelectrics and dielectrics (XVII NSFD-2012) held during 17th-19th December 2012 at Institute of Technical Education and Research (ITER), Bhubaneswar, Odisha.
7. "Design and analysis of Solidly Mounted Resonator utilising a conductive Bragg reflector to improve Q and resonant frequency", Amsanpally, A.; Enjamuri, S.; **K.C.James Raju.**, presented at "5th International conference on Computers and Devices for Communication", held during 17-19, December, 2012 at Institute of Radio Electronics, Kolkota.
8. "Application of PSO Algorithm for Optimizing the Dimensions of Tunable Interdigitated Capacitor", G. Lakshmi Narayana Rao, Sravan Kumar, Samrat L. Sabat, and **K. C. James Raju**, PIERS Proceedings, Progress In Electromagnetics Research Symposium Proceedings, KL, MALAYSIA, 2012, pp.1401-1406.
9. "Fabrication of High Dielectric Constant and Low Loss X Band Ceramic Waveguide Window for High Power Applications." S.Bashaiah, Pramod

- K.Sharma and **K.C.James Raju**, 5th International conference on Computers and Devices for Communication," CODEC.2012.6509286, Publication Year: 2012 , Page(s): 1 – 4.
10. "Vertical interconnect modeling between GCPWs in LTCC technology," Pavan, C.L.N.; **K.C.James Raju**; *Microelectronics and Electronics (PrimeAsia), 2012 Asia Pacific Conference on Postgraduate Research in* , pp.211-213, 5-7 Dec. 2012, doi: 10.1109/PrimeAsia.2012.6458656.
 11. "Design of resonator based ultra wideband bandpass filter in Low Temperature Cofired Ceramic Technology", C H L N Pavan, **K.C.James Raju**, " Proceedings of 5th IEEE International Conference on Computers and Devices for Communication (CODEC), 2012, vol., pp.1-3, 17-19 Dec. 2012, doi: 10.1109/CODEC.2012.6509287.
 12. "Design and analysis of Solidly Mounted Resonator utilising a conductive Bragg reflector to improve Q and resonant frequency," Amsanpally, A.; Enjamuri, S., **K.C.James Raju**., Computers and Devices for Communication (CODEC), 2012 5th International Conference on, pp.1-4, 17-19 Dec.2012. doi: 10.1109/CODEC.2012.6509281.

Publications (acknowledging CMSD): S. Mahapatra [2012-2013(March)]

S No	Authors	Title	Journal, volume, page No. and year
11.	T. Rajagopala Rao and S. Mahapatra	Theoretical study of CIH2- electron detachment spectroscopy revisited	Chem. Phys. Lett. 574, 24-31 (2013)
10	T. Rajagopala Rao, S. Goswami, S.Mahapatra , B. Bussery-Honvault and P. Honvault	Time-dependent quantum wave packet dynamics of the C+OH reaction on the excited electronic state	J. Chem. Phys. 138, 094318 (1-10) (2013).
9	T. Mondal, S. Rajagopala Reddy and S. Mahapatra	Photophysics of fluorinated benzene. III. Hexafluorobenzene	J. Chem. Phys. 137, 054311(1-17) (2012).

8	T. Roy and S. Mahapatra	Quantum dynamics of H+LiH reaction and its isotopic variants	J. Chem. Phys. 136, 174313(1-12) (2012).
7	S. Nagaprasad Reddy and S. Mahapatra	Theoretical study of electronic absorption spectroscopy of propadienylidene molecule vis-à-vis the observed diffuse interstellar bands	Chem. Phys. 403, 1-11 (2012)
6	S. Rajagopala Reddy and S. Mahapatra	Theoretical study of photodetachment processes of anionic boron clusters .II. Dynamics	J. Chem. Phys. 136, 024323(1-13) (2012).
5	S. Rajagopala Reddy and S. Mahapatra	Theoretical study of photodetachment processes of anionic boron clusters .I. Structure	J. Chem. Phys. 136, 024322(1-15) (2012).
4	S. Ghanta, V. S. Reddy and S. Mahapatra	Theoretical study of electronically excited radical cations of naphthalene and anthracene as archetypal models for astrophysical observations. II. Dynamical consequences	Phys. Chem. Chem. Phys. 13, 14531-14541 (2011).
3	S. Ghanta, V. S. Reddy and S. Mahapatra	Theoretical study of electronically excited radical cations of naphthalene and anthracene as	Phys. Chem. Chem. Phys. 13, 14523-14530 (2011).

		archetypal models for astrophysical observations. I. Static aspects	
2	T. R. Rao and S. Mahapatra	Nuclear motion on the orbitally degenerate electronic ground state of fully deuterated triatomic hydrogen	J. Chem. Phys. 134, 204307 (1-16) (2011).
1	Tanmoy Roy, T. Rajagopala Rao and S. Mahapatra	Quantum dynamics of H + LiH ⁺ reaction on its electronic ground state	Chem. Phys. Lett., 501, 252-256 (2011).

(Prof. V.S.S. Sastry)

Information for Annual Report – 2013 for CMSD

Lecture delivered elsewhere on invitation - under Chapter 12:

Invited Lecture: “Phase Diagram of the Quadratic Hamiltonian of Biaxial Molecules: New Insights from Monte Carlo Simulations”, 18th December, 2012, at Raman Research Institute in Bangalore.

Invited Talk in a Conference - under Chapter 13:

Invited Talk: “Phase Transitions in Biaxial Nematics : Mean-field Theoretic Expectations and Monte Carlo Predictions”, on 11th January, 2013, at the *Conference on Condensed Matter and Biological Systems* (CCMB13) held in Department of Physics, Banaras Hindu University in Varanasi.

Papers presented in a Conference - under Chapter 13:

2. Paper: “Rare biaxial fluctuations in uniaxial nematic phase: Monte Carlo simulation study”, presented by Regina Jose, D. Jayasri, K.P.N. Murthy and V.S.S. Sastry, in the *International Liquid Crystal Conference (ILCC)* held in Mainz, Germany, August 19-24, 2012
3. Paper: “Rare microstates in a biaxial nematic system: Novel Monte Carlo study”, presented by Regina Jose, D. Jayasri, K.P.N. Murthy and V.S.S. Sastry, in 19th *National Conference on Liquid Crystals (NCLC-19)* held in the Thapar University, Patiala, November 21-23, 2012.
4. Paper: “Monte Carlo study of Pretransitional behaviour of a biaxial nematic with variation of molecular biaxiality”, presented by B. Kamala Latha, Regina Jose, K.P.N. Murthy, V.S.S. Sastry, in 19th *National Conference on Liquid Crystals (NCLC-19)* held in the Thapar University, Patiala, November 21-23, 2012.
5. Paper: “Simulations of phase transitions in Hybrid Planar films of Biaxial liquid crystals”, presented by B. Kamala Latha, G. Sai Preeti, N. Satyavathi, K.P.N. Murthy and V.S.S. Sastry, in 19th *National Conference on Liquid Crystals (NCLC-19)* held in the Thapar University, Patiala, November 21-23, 2012.
6. Paper: “Exploring rare microstates in a biaxial system using an order-parameter based entropic sampling method”, presented by Regina Jose, D. Jayasri, K. P. N. Murthy and V. S. S. Sastry; in the *Conference On Condensed Matter and Biological Systems (CCMB13)*, held in the Banaras Hindu University, Varanasi, January 11-14, 2013.
7. Paper: “Defects in Biaxial Nematic Films : Monte Carlo Simulations”, presented by G. Sai Preeti, C. Chiccoli, P. Pasini, C. Zannoni, and V.S.S. Sastry, in the *Conference on Condensed Matter and Biological Systems (CCMB13)*, held in the Banaras Hindu University, Varanasi, January 11-14, 2013.

Published papers (Chapter 14):

1. *On defects in biaxial nematic films with random planar surface alignment: A Monte Carlo study*, G. Sai Preeti, C. Chiccoli, P. Pasini, V.S.S. Sastry and C. Zannoni, *Mol. Cryst. Liq. Cryst.*, **573**, 10 (2013)

2. *Lattice spin simulations of topological defects in biaxial nematic films with homeotropic surface alignment*, G. Sai Preeti, C. Zannoni, C. Chiccoli, P. Pasini, and V.S.S. Sastry, *Int. J. Mod. Phys. C* **24**, 1350026 (2013)

Ongoing project(s) - Chapter 15:

1. DST sponsored project on *Computer Simulations and NMR Investigations of Responsive Materials for Photonics Applications*, under Indo-Italian Joint Collaboration scheme, with Professor Claudio Zannoni of the University of Bologna, Bologna, Italy, from June 2012 for three years:

Seminars and Workshops conducted:

1. CMSD and Centre for Development of Advanced Computing are Jointly Conducted a Technology Workshop on Heterogeneous Computing - CPU/GPU HPC Cluster Algorithms & Performance of Application Kernels during July 16-20, 2012 at CMSD, University of Hyderabad.
2. The National MEMS Design Centres of UOH and OU are Jointly Conducted MEMS Design - Training Workshop during August 6-11, 2012 at CMSD, University of Hyderabad.
3. University of Hyderabad, National Institute of Animal Biotechnology(NIAB), CR Rao AIMSCS and CCMB are Jointly Conducted a Workshop on Genomics & Beyond during December 6-16, 2012 at CMSD, University of Hyderabad.
4. Department of Biotechnology Conducted a Workshop on Programming on R and Applications in Computational Biology during January 10-13, 2013 at CMSD, University of Hyderabad.
5. Centre for Neural & Cognitive Sciences is Conducted Indo-Italian Training Workshop on EEG & MEG DATA PROCESING during April 1-4, 2013 at CMSD, University of Hyderabad.
6. Dr. Shoibal Chakraborty of Princeton University delivered a lecture on "Open source models and the development of associated website/computational infrastructure" on 16th November 2012.

Dr. Siba K Udgata is the Director of the CMSD. Prof. V S S Sastry is Resource Coordinator and Prof. K P N Murthy is Academic Coordinator.

