Annual Report
2011-2012

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 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 Ensight Application Software
- Remote Visualization Software Single User

Adjunct Professor

1. Prof. Claudio Zannoni, Dipartimento di Chimica Fisica Ed Inorganica, Universita di Bologna, Italy, (February 18, 2009 to February 17, 2011).
2. Prof. Anil Kumar, Dept. of Physics & NMR Research Centre, Indian Institute of Science (June 20, 2009 to June 19, 2012)

Visiting Professor

1. Dr. Debasis Chakraborty, Scientist 'G', Directorate of Computational Dynamics, DRDL, Hyderabad
2. Dr. M R Reddy, Metabasis Therapeutics, San Diego, USA.
3. Dr. Ingua Ramarao, Computational Physicist, East West Enterprises Inc., USA
4. Prof.K.V.Subba Rao, UCESS, University of Hyderabad, Hyderabad

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

Mr.Amit Singh, recipient of UGC Dr. D. S. Kothari Postdoctoral Fellowship has joined CMSD on September 2011, for a period of 3 years.

Papers Published from CMSD:

1. Siva Nasarayya chari, K P N Murthy and Inguva Ramarao, *A study of non-equilibrium work distributions from fluctuating lattice Boltzmann model,* Physical Review **E 85**, 041117 (2012).
2. N. Shankaraiah, K P N Murthy, T. Lookman, and S.R. Shenoy, *Conversion times and energy/entropy barriers in isothermal/athermal martensites,* Journal of Alloys and Compounds, Available online 17 March 2012
3. N. Shankaraiah, K P N Murthy, T. Lookman, and S. R. Shenoy, *Monte Carlo simulations of strain pseudospins: Athermal martensites, incubation times, and entropy barriers*, Physical Review B **84**, 064119 (2012)
4. M. Ponmurugan, V. Sridhar, and S.L. Narasimhan, and K P N Murthy, *flatIGW - An inverse algorithm to compute the density of states of lattice self avoiding walks,* Physica A: Statistical Mechanics and its Applications, **390**, 1258 (2011).
5. M. Suman Kalyan, G. Anjan Prasad, V.S.S. Sastry, and K P N Murthy, *A note on non-equilibrium work fluctuations and equilibrium free energies,* Physica A: Statistical Mechanics and its Applications, **390**, 1240 (2011).
6. Rajagopala Rao and S. Mahapatra, Nuclear motion on the orbitally degenerate electronic ground state of fully Deuterated triatomic hydrogen T, *J. Chem. Phys.* **134**, (20), 4307 (2011)

7. D. Jayasri, T. Sairam, K. P. N. Murthy and V. S. S. Sastry , Liquid crystal films on curved surfaces: An entropic sampling study**,** *physica A (communicated),* (2011)

8. Tapta Kanchan Roy and M. Durga Prasad, Development of a new variation approach for thermal density matrices, *J. Chem. Phys.* **134**, 214110 (2011)
9. Subhendu Roy, Eluvathingal D. Jemmis, Martin Ruhmann, Axel Schulz, Katharina Kaleta, Torsten Beweries, and Uwe Rosenthal, Theoretical Studies on the Structure and Bonding of Metallacyclocumulenes, - Cyclopentynes and –cycloallenes, *Organometallics*, 2011, 30 (10), pp 2670–2679

10. R.S. Rathore, P. Aparoy, P. Reddanna, A. K. Kondapi, M. Rami Reddy, Minimum MD simulation length required to achieve reliable results in free energy perturbation

calculations: Case study of relative binding free energies of fructose-1,6-bisphosphatase inhibitors, *Journal of Computational Chemistry* 32, **(10)**, 2097–2103, (2011)

11. P. Aparoy, G. K. Suresh, K. Kumar Reddy, P. Reddanna, CoMFA and CoMSIA studies on 5-hydroxyindole-3-carboxylate derivatives as 5-lipoxygenase inhibitors: Generation of homology model and docking Studies, *Bioorganic & Medicinal Chemistry Letters,* 21, (1), 2011, 456-462

12. N. Yedukondalu, K. Ramesh Babu, Ch. Bheemalingam, David J. Singh, G. Vaitheeswaran, and V. Kanchana, Electronic structure, optical properties, and bonding in alkaline-earth halo fluoride Scintillations: BaClF, BaBrF, and BaIF, *Phys. Rev.* **83**, 165117 (2011) [7 pages]

13. Rafiya Sultana, Karunakar Tanneeru, Lalitha Guruprasad, The PE-PPE Domain in Mycobacterium Reveals a Serine a/b Hydrolase Fold and Function: An In-Silico Analysis *PLoS ONE*, **6**, (2), e16745, (2011)

14. Kunduchi P. Vijayalakshmi, Neetha Mohan, Manjaly J. Ajitha and Cherumuttathu H. Suresh, Mechanism of epoxide hydrolysis in microsolvated nucleotide bases adenine,Guanine and cytosine: A DFT study, *The Royal Society of Chemistry 2011*

15. Ch. Bheema Lingam, K. Ramesh Babu, Surya P. Tewari, G. Vaitheeswaran **,** Structural, electronic, bonding, and elastic properties of NH_3BH_3: A density functional Study, *Journal of Computational Chemistry* 32**, (8),** 1734–1742, (2011)

16. K. Ramesh Babu, Ch. Bheema Lingam, Surya P. Tewari and G. Vaitheeswaran, High-Pressure Study of Lithium Azide from Density-Functional Calculations, *J Phys Chem A.* 2011 May 5;115(17):4521-9. Epub 2011 Apr 12.

17. Sachin D. Yeole and Shridhar R. Gadre, Molecular cluster building algorithm: Electrostatic guidelines and molecular Tailoring approach, J. Chem. Phys. **134**, 084111 (2011)

18. A.R. Biju and M.V. Rajasekharan Structure, magnetic properties, catalase activity and DFT studies of $[Mn_2(\mu-RCOO)_2(\mu-OR)_2]^{2+}$ Type Dinuclear manganese (III, III) complexes *Inorganica Chimica Acta* 372, (1), 2011, 275-280

19. N Suman Kalyan, Anjan Prasad, V S S Sastry and K P N Murthy, A note on non-equilibrium work fluctuations and equilibrium free energies, Physica A (2011) doi:10.1016/j.physa.2010.11.018

20. Ch. Bheema Lingam, K. Ramesh Babu, Surya P. Tewari, G. Vaitheeswaran, and S. Lebègue, Quasiparticle band structure and optical properties of NH3BH3, Phys. Status Solidi RRL 5, No. 1, 10 – 12 (2011) / DOI 10.1002/pssr.201004432

21. Regina Jose, D. Jayasri, Surajit Dhara, K. P. N. Murthy and V. S. S. Sastry, Effect of external field on the nematic to isotropic transition: an entropic sampling study, *Mol. Cryst. Liq. Cryst.,* **545**, 168 (2011).

22. B. Kamala Lata, G. Sai Preeti, N. Satyavathi, K.P.N. Murthy, and V.S.S. Sastry, Anchoring transitions in biaxial nematic droplets: A Monte Carlo Study, *Mol. Cryst. Liq. Cryst.,* **545**, 230 (2011)

Prof. K. P. N. Murthy

Invited Lectures:

1. Resource Person, in Science Academies' Refresher course on Statistical Mechanics, 30 April to 12 May, 2012, at Nehru Arts and Science College, Kanhangad

2. Invited Lectures: *Statistical Mechanics – I, and II*, in Science Academies ' Lecture Workshop on Fundamental Concepts in Basic Physics for Master Course Students and Teachers, Department of Physics, P S G R Krishnammal College for Women, Coimbatore, 5 - 6, January 2012.

3. Invited talk, on 13 March 2012, on *Simulation of a switching experiment on an ideal gas using fluctuating lattice Boltzmann model,* Conference on Statistical Physics and Non-linear Dynamics (CSPND), 12-16, March 2012, S N Bose National Centre for Basic Sciences, Kolkatta

4. Invited talk, *Boltzmann and non-Boltzmann Monte Carlo*, First Annual Symposium on Current Trends in Computational Natural Sciences (CT - CNS 2012) February 26, 2012, International Institute of Information Technology (IIIT) Hyderabad

5. Invited talk, *Entropy then and entropy now*, School of Physics, Mizoram Central University, June 8, 2012.

6. Invited Lectures, *Statistical ensembles - I, II and III*, in the Lecture Workshop on Statistical Mechanics, Organized by the Academy of Sciences, Bangalore, in Department of Physics, Nehru Arts and Science College, Kanhangad, 15 - 17, July 2011.

7. Invited Seminar, *Demons don't die*, Alabama A & M University, Huntsville, Alabama, 13 June 2011

8. Special Lecture, *Daniel Bernoulli and his fluid dynamics*, 23 December 2011, in Advanced Instructional School on Mechanics, Department of Mathematics, University of Hyderabad 5 - 24 December 2011.

9. Special Lecture, *Laws of thermodynamics*, , 24 December 2011 in Advanced Instructional School on Mechanics, Department of Mathematics, University of Hyderabad 5 - 24 December 2011

10. Special Lecture, *Lattice Boltzmann, non-equilibrium work and equilibrium free energies,* 15 December 2011, in DST-SERC School on Nonlinear Dynamics, IISER, Pune, 4 - 24, December 2011.

11. Invited talks: Demonstration and hands-on practice sessions *on regular and anomalous diffusion, random walks, Levy walks, rejection and Metropolis rejection techniques, and Langevin equations*, 16 - 17 December 2011, in DST-SERC School on Nonlinear Dynamics, IISER, Pune, 4 - 24, December 2011

12. .Invited lectures and tutorial sessions on *Monte Carlo - then and Monte Carlo - now*, in the theme meeting on Diffusion, mass transfer and its consequences in materials, Structure and thermodynamics of emerging materials : STEM - 2011, Convention Center, Anupuram, November 24 - 26, 2011.

Research Papers:

1. Siva Nasarayya Chari and K. P. N. Murthy, *Non-Equilibrium work distributions from fluctuating lattice-Boltzmann model,* Frontiers in Physics, School of Physics, University of Hyderabad, 28 - 29 October 2011.
2. N Shankaraiah, K. P. N. Murthy, T Lookmann, and S R Shenoy, *Microstructures and conversion delays in martensites: Monte Carlo study of strain pseudo spin models*, Frontiers in Physics, 28 - 29 October 2011, School of Physics, University of Hyderabad.
3. Ch Sandhya, K Hima Bindu, K. P. N. Murthy, and V S S Sastry, *Phase transition in a bond fluctuactuating linear homo polymer*, American Institute of Physics Conference Proceedings, 1349, 117 (2011).
4. S C R Roshan, Lavanya Kunduru, Regina Jose, K. P. N. Murthy, and V S S.Sastry, *Azimuthal biaxiality in patterned nematic liquid crystal films : A Monte Carlo Study*, American Institute of Physics Conference Proceedings, 1349, 178 (2011).
5. Lavanya Kunduru, S C R Roshan, B K Latha, K. P. N. Murthy, and V S S.Sastry, *Polymer network induced ordering in biaxial nematic liquid crystals :a Monte Carlo study*, American Institute of Physics Conference Proceedings,1349, 182 (2011).

Books:

1. (with D Jayasri and V S S Sastry), *Monte Carlo Studies of Liquid Crystalline Systems,* LAP Lambert Academic Publishing (2011).
2. (with Siva Nasarayya chari and Inguva Ramarao), *A study of non-equilibrium work distributions from fluctuating lattice Boltzmann model,* Physical Review **E 85**, 041117 (2012).
3. (with N. Shankaraiah, T. Lookman, and S.R. Shenoy), *Conversion times and energy/entropy barriers in isothermal/athermal martensites,* Journal of Alloys and Compounds, Available online 17 March 2012
4. (with Gunter Schuetz), *Mean bubble formation time in DNA denaturation*, EurophysicsLetters **96**, 68003 (2011).
5. (with N. Shankaraiah, T. Lookman, and S. R. Shenoy), *Monte Carlo simulations of strain pseudospins: Athermal martensites, incubation times, and entropy barriers*, Physical Review B **84**, 064119 (2011)
6. (with Gouripeddi Sai Preeti, and V. S. S. Sastry, Cesare Chiccoli, Paolo Pasini,Roberto Berardi and Claudio Zannoni), *Does the isotropic - biaxial nematic transition always exist? A new topology for the biaxial nematic phase diagram,* Soft Matter **7**, 11483 (2011).
7. (with D. Jayasri, T. Sairam, and V.S.S. Sastry), *Liquid crystal films on curved surfaces: An entropic sampling study Physica A: Statistical Mechanics and its Applications* **390**, 4549 (2011)

8. (with M. Ponmurugan, V. Sridhar, and S.L. Narasimhan), *flatIGW - An inverse algorithm to compute the density of states of lattice self avoiding walks,* Physica A: Statistical Mechanics and its Applications, **390**, 1258 (2011).
9. (with M. Suman Kalyan, G. Anjan Prasad, and V.S.S. Sastry), *A note on non-equilibrium work fluctuations and equilibrium free energies,* Physica A: Statistical Mechanics and its Applications, **390**, 1240 (2011).
10. (with Regina Jose, D. Jayasri, Surajit Dhara, and V. S. S. Sastry), *Effect of External Field on the Nematic to Isotropic Transition: An Entropic Sampling Study*, Molecular Crystals and Liquid Crystals **545**, 168/[1392] (2011).
11. (with B. Kamala Latha, G. Sai Preeti, N. Satyavathi, and V. S. S. Sastry) *Anchoring Transitions in Biaxial Nematic Droplets: A Monte Carlo Study*,Molecular Crystals and Liquid Crystals **545**, 230[1454] (2011)

Dr. Cherumuttathu H. Suresh

1. Sayyed, F. B.; Suresh, C. H. Accurate prediction of cation-pinteraction energy using substituent effects *J.Phys.Chem.A* **2012,** 116, 5723.
2. Vijayalakshmi, K. P.; Mohan, N.; Ajitha, M. J., Suresh, C. H. Mechanism of epoxide hydrolysis in microsolvated nucleotide bases
   adenine, guanine and cytosine: A DFT study *Org. Biomol. Chem*. **2011**, 9, 5115.

3. Mathew, J., Suresh, C.H. Assessment of steric and electronic effects of N-heterocyclic carbenes in grubbs olefin metathesis using
   molecular electrostatic potential *Organometallics* **2011,** 30, 3106.

Dr. Satyen Saha

1. M. Shukla, N. Srivastava, S. Saha, Theoretical and spectroscopic studies of 1-butyl-3-methylimidazolium iodide room temperature ionic liquid: Its differences with chloride and bromide derivatives, Journal of Molecular Structure 975 (2010) 349–356.

2. M. Shukla, N. Srivastava, S. Saha , T.R. Rao, S. Sunkari, Synthesis, structure, UV–Vis–IR spectra, magnetism and theoretical studies on CuII[(2-aminomethyl)pyridine](thiocyanate)2 and comparisons with an analogous CuII complex, Polyhedron 30 (2011) 754–763.

3. M. Shukla, N. Srivastava, S. Saha, Investigation of ground state charge transfer complex between paracetamol and p-chloranil through DFT and UV–visible studies, Journal of Molecular Structure 1021 (2012) 153–157.

Dr. Lalitha Guruprasad

1. Srinivas Nakka and Lalitha Guruprasad. The imidazolidone analogs as phospholipase D1 inhibitors: analysis of the three-dimensional quantitative structure-activity relationship. Medicinal Chemistry Research, 2011, DOI: 10.1007/s00044-011-9773-3.

2. Srinivas Nakka, Lalitha Guruprasad. Structural Insights into the Active Site of Human Sodium Dependent Glucose Co-Transporter 2: Homology Modelling, Molecular Docking, and 3D-QSAR Studies. Australian Journal of Chemistry, 2012, DOI: 10.1071/CH12051.

3. Karunakar Tanneeru & Lalitha Guruprasad. Ligand-based 3-D pharmacophore generation and molecular docking of mTOR kinase inhibitors. J. Mol. Model. (2012) 18:1611-1624.

4. Karunakar Tanneeru, Bandi Madhusudhan Reddy, Lalitha Guruprasad. Three-dimensional quantitative structure–activity relationship (3D-QSAR) analysis and molecular docking of ATP-competitive triazine analogs of human mTOR inhibitors. Medicinal Chemistry Research (2012),21: 1207-1217.

5. Angamba Meetei Potshangbam, Karunakar Tanneeru, Bandi Madhusudhan Reddy, Lalitha Guruprasad. 3D-QSAR and molecular docking studies of 2-pyrimidinecarbonitrile derivatives as inhibitors against falcipain-3.Bioorganic & Medicinal Chemistry Letters (2011) 21: 7219-€"7223.

6. Rafiya Sultana, Karunakar Tanneeru, Lalitha Guruprasad. The PE-PPE Domain in Mycobacterium Reveals a Serine a/b Hydrolase Fold and Function: An In-Silico Analysis. PLoS ONE 6(2): e16745. doi:10.1371/journal.pone.0016745

Prof. VSS Sastry

Journal Publications:

1. G Saipreeti, K. P. N. Murthy, C. Chicolli, C. Zannoni, V. S. S. Sastry, *Does the isotropic-biaxial nematic transition always exist ? A new topology for the biaxial nematic phase diagram*, *Soft Matter* **7**, 11483 (2011).

2. D. Jayasri, T. Sairam, K. P. N. Murthy, and V. S. S. Sastry, *Liquid crystal films on curved surfaces: An entropic sampling study*, *Physica* **A 390**, 4549 (2011)

3. Ch Sandhya, K Hima Bindu, K. P. N. Murthy and V S S Sastry, *Phase transition in a bond fluctuating linear homo polymer*, AIP Conf. Proc. **1349**, 117 (2011).

Book:

1. D Jayasri, V S S Sastry and K P N Murthy, *Monte Carlo Studies of Liquid Crystalline Systems*, LAP Lambert Academic Publishing, Germany (2011)

Conference papers:

1. *K. Kamala Latha , N. Satyavathi , K.P.N. Murthy and V.S.S. Sastry, Exploration of tricritical regions in the biaxial nematic phase diagram: Application of Monte Carlo simulations,* XIX Conference on Liquid Crystals*, September 2011, Międzyzdroje, Poland

2. *G. Shwetha, K.P.N. Murthy, and V.S.S. Sastry, Monte Carlo simulation of thermally induced SmCP phases of bent-core liquid crystals in an applied field*, XIX Conference on Liquid Crystals*, September 2011, Międzyzdroje, Poland

DR. K C JAMES RAJU

PAPERS PUBLISHED (in refereed Journals)

1. Tunable Interdigital Capacitors with$Ba0.5Sr0.5TiO3$ Thin Films on Low-k Substrates for Frequency Agile Microwave Devices, G. Laxmi Narayana Rao, K. Venkata Saravanan, K.C. James Raju, Integrated Ferroelectrics, **125**, 2011, pp.20-28.

Refereed Proceedings and Book Chapters

1. 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, pp.1401 – 1406.

Conference Presentations:

1. High dielectric constant and low loss X band Ceramic Waveguide Window for selective frequencies, S. Bashaiah , K. C. James Raju , Frontiers in Physics, October 28-29, UOH, Hyderabad.

2. Optimization and analysis of piezoelectric and electrode materials thickness effects on the performance of film bulk acoustic resonator, Srikanth Enjamuri, Abhilash Amsanpally, K.C. James Raju, IEEE Conference ISPTS-2012, 8-12, March, 2012 at Pune.

3. Self Aligned MEMS Based High-Q Disk Resonator, Vikram Kumar Singh, Abhilash Amsanpally, K.C. James Raju, IEEE Conference ISPTS-2012, 8-12, March, 2012 at Pune.

4. "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, Progress in Electromagnetics Research Symposium, (PIERS 2012), 27-30, March 2012, Kuala Lumpur, Malaysia.

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.