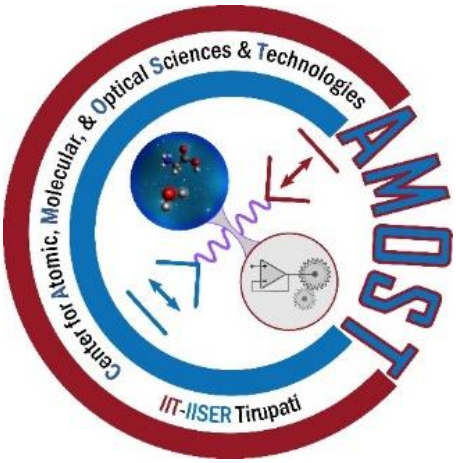
ABOUT CAMOST



Center for Atomic, Molecular, & Optical Sciences & Technologies (CAMOST)

A JOINT INITIATIVE OF IIT TIRUPATI & IISER TIRUPATI

भारतीय प्रौद्योगिकी संस्थान तिरुपति

TIRUPATI

IISER
TIRUPATI

About CAMOST

AMO (Atomic, Molecular, and Optical) sciences encompass significant areas of human activities directly impacting life through applications in health, communication, navigation, metrology, space, internet and quantum technologies. Advances in the field of quantum computing would lead to exciting possibilities in solving problems related to weather modeling, evolution of our Universe, secure communication, etc.

Tirupati is the only town in India which is home to both an Indian Institute of Technology (IIT) and an Indian Institute of Science Education and Research (IISER). These two institutes started together at Tirupati in 2015 and have leveraged each other's unique strengths by sharing resources, and have now come together to establish the Center for Atomic, Molecular, & Optical Sciences & Technologies (CAMOST) to address key challenges in frontier areas of AMO sciences and technologies. Researchers from institutions pan-India would collaborate with each other under the aegis of CAMOST.

CAMOST is India's first such center in a University environment where some of the country's best undergraduate and graduate students interact closely with post-doctoral researchers and distinguished faculty. Close cooperation between scientists and engineers from IIT Tirupati, IISER Tirupati and also from several other premier institutes in India would come under CAMOST's initiatives. This partnership is already nucleated and the formal inauguration of CAMOST takes place at the hands of Dr Arabinda Mitra (Scientific Secretary, Office of the Principal Scientific Advisor, Government of India) on August 14th, 2020, on the eve of the 73rd anniversary of the India's INDEPENDENCE DAY.

Vision

Inspire tangible solutions to frontier problems in AMO Science and Technologies through innovative research initiatives in basic and applied science domains.

Mission

To advance the field of AMO Sciences and Technologies by:

- Developing innovative solutions to frontier problems of AMO Quantum Science and Technology
- Contributing to solving key problems in atmospheric, space, and bio sciences
- Fostering human resources to meet 21st century challenges in AMO quantum Sciences & Technologies

Thrust Areas

- Ultrafast physics: Quantum dynamics on attosecond time scale
- Quantum communication and Quantum technology applications
- Quantum photonics: Cold plasma applications
- Laboratory astrophysics, Astrochemistry, and Atmospheric Sciences
- Optical tweezers for biomedical applications
- Single molecule magnetism for high-density data storage
- Quantum Chemistry and Statistical Mechanics
- High Technology Devices

Joint Initiatives of IIT Tirupati & IISER Tirupati in AMO Sciences and Origin of CAMOST

IIT Tirupati and IISER Tirupati have been constructively sharing their resources, including faculty, to leverage each other's strengths. Below is a list of few initiatives in which both the institutes worked closely together, the latest of which marked the establishment of CAMOST.

1. **The 7th Topical Conference (TC7) of the Indian Society of Atomic and Molecular Physics (ISAMP)** was held under the joint auspices of the IIT Tirupati and IISER Tirupati from 6th to 8th January 2018.
   Conveners: P C Deshmukh and Bhas Bapat; Conference Secretary: S Sunil Kumar
   Proceedings of the Conference have been published by Springer (2019), under the title 'Quantum Collisions and Confinement of Atomic and Molecular Species, and Photons'
   Editors: P C. Deshmukh, E. Krishnakumar, S Fritzsche, M Krishnamurthy, and S. Majumder
   ISAMP-TC7 was attended by well over a hundred participants including many from abroad.
2. **Deliberations in Atomic Physics (DAP)**: A new seminar-cum-discussion series, DAP was launched in March 2018. This consisted of a 2-Days Workshop on ULTRAFAST and MANY-BODY ATOMIC PHYSICS, and was held at IIT Tirupati on 8th and 9th March 2018.
   DAP was attended by select invited participants from IIT Delhi, PRL Ahmedabad, IIT Madras, IISER Tirupati, IIT Mandi, IIT Patna, IIT Roorkee, GCE Gaya, and GSU USA.
3. **Establishment of CAMOST**: One-day symposium was held on 20th March 2019 when some senior AMO scientists and several young scientists from various places in India met at IIT Tirupati to discuss the formation of the CAMOST at Tirupati.
   Convener: P C Deshmukh
   Presided by: K N Satyanarayana (Director, IIT Tirupati) and K N Ganesh (Director, IISER Tirupati)
   Attendees:
   S T Manson (GSU, USA)
   E Krishnakumar (RRI, Bengaluru)
   Dilip Angom (PRL, Ahmedabad)
   C P Safvan (IUAC, New Delhi)
   G Ambika (IISER Tirupati)
   S Sivakumar (KREA University)
   Arijit Sharma, Reetesh Gangwar, Vinay P Majety (IIT Tirupati)
   S Sunil Kumar, Soumit Mandal (IISER Tirupati)
   Koushik Saha (IIT Dharwad), Rajesh K Kushawaha (PRL, Ahmedabad)
   Sivarama Krishnan (IIT Madras), Dhananjay Nandi (IISER Kolkata)

   Senior AMO scientists emphasized the urgent need for having such a national resource to be set up and expressed happiness that such a center is now realizable due to the vision of the Directors of IIT Tirupati and IISER Tirupati, crystallizing the long standing aspirations of AMO scientists in the country. The special opportunity at Tirupati was recognized considering the significant pool of young faculty at IIT Tirupati and IISER Tirupati who specialized in AMO sciences. E Krishnakumar, Dilip Angom and C P Safvan submitted detailed reports recommending the formation of CAMOST at Tirupati.

Administrative Council

K N Satyanarayana
Director, IIT Tirupati

K N Ganesh
Director, IISER Tirupati

Mentor & Convener

P C Deshmukh
Adjunct Professor, IIT Tirupati

Scientific Advisory Council

Dilip Angom
PRL, Ahmedabad

E Krishnakumar
RRI, Bangalore

C P Safvan
IUAC, New Delhi
(President of ISAMP)

Dmitry Budker
JGU Mainz & UCB

John Costello
Dublin City University

Bhanu Pratap Das
Tokyo Institute of Technology

S T Manson
Georgia State University

G Ravindrakumar
TIFR, Mumbai

Roland Wester
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MPI for Complex Systems

Core Administrative Members

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G Ambika
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Soumit Mandal

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PRL, Ahmedabad

S Sivakumar

KREA University

Sivarama Krishnan

IIT Madras

Ramachandra R Yalla

University of Hyderabad

G V Pavan Kumar

IISER Pune

PHASE I Proposals by CORE GROUP SCIENTISTS at CAMOST from IIT Tirupati and IISER Tirupati

Deshmukh, P.C.

[1] Study of time, and time-delay, in quantum phenomenology.

Time is not an observable; time-delay is. Our research group is engaged in a phenomenological study of the role of time-delay in ultrafast processes in atoms and ions on the attoseconds time scale. We develop sophisticated models using relativistic many-body theory. The results are of importance in many technologies, including calibration of atomic clock.

[2] Relativistic and electron-correlations effects in atomic photoabsorption processes in atoms and ions.

We employ the Relativistic Random Phase Approximation (with, and without relaxation), The Relativistic Multichannel Tamm-Dancoff, and the Relativistic Multichannel Quantum Defect Theory to investigate complex atomic spectra from small, medium, heavy and superheavy atoms and ions. Our investigations include the analysis of the spectral regions in which sensitive autoionization takes place.

[3] Applications of the Lambert W function in pure and applied physics, especially in the domain of quantum theory of atoms, molecules on the nano-scale.

We are engaged in exploiting the powers of methods in complex analysis, conformal mappings etc. to seek analytical solutions to problems for which only numerical or graphical solutions were hithert available. These provide fruitful insights into the dynamics of physical processes.

Gangwar, Reetesh Kumar

The cold plasma science and technology has emerged with promising potentials for the plethora of issues in various areas such as material processing, medicine, agriculture, food processing, environmental remediation etc. The prime attraction in using these plasmas lies in their unique ability to offer a cocktail of reactive species at room temperature. One of the major challenges with cold plasma technology is to make it economically viable which requires a deep understanding of plasma-liquid interactions. Our research group at IIT Tirupati is involved in performing the characterization of cold plasma systems by coupling of optical emission measurements with the collisional radiative models. Expertise in atomic & molecular physics and plasma physics is essential to implement this scheme. Such expertise is very limited in INDIA. Dr. Gangwar has experience and expertise in developing cold plasma systems and thereafter performing the plasma-characterization using spectroscopic techniques. Currently, we are focusing on following research areas

- Development of flexible cold atmospheric pressure plasma reactor for direct and indirect treatment
- Cold Plasma mediated wastewater treatment
- Cold plasma for pre- and post-harvest treatment
- Development cold plasma jets for plasma-mediated ionization of biological samples

Majety, Vinay P.

First principles modeling of quantum dynamics at attosecond time scale in atoms and molecules

The current generation of high harmonic generation based attosecond light sources and free electron lasers have the potential to probe electronic motion on its natural time scale. Our goal is to develop novel many body techniques that can accurately model the interaction of atoms and molecules with these state of the art ultrashort light pulses and employ them to explore various pump-probe schemes that could unravel correlated quantum dynamics on their natural time scale.

Mandal, Soumit

Single molecule force spectroscopy of macromolecular systems

Biophysics correlate structure and conformational changes of biomacromolecules with their functions. DNA Biophysics represents one such exciting system. DNA intercalation represents an invasive and reversible mode of DNA-ligand binding. DNA intercalation allow a wide range of therapeutic applications. Many anticancer drugs in clinical use interact with DNA with transfer of the intercalating molecule from an aqueous environment to the hydrophobic space between DNA base pairs. Minor groove binding proteins interact with DNA to create bend structures. Conformational changes in DNA and protein during this interaction is debated. The mechanism by which protein intercalates into DNA leading to changes in their structure is unknown as the changes occur in fast time scales. In this project, we plan to use optical tweezer to study protein-DNA interaction. High spatial and temporal resolution will enable us to first identify short-lived intermediate states generated when the protein intercalates to DNA and finally propose a kinetic pathway. These experiments can serve as an assay for screening of drugs. The short-lived intermediate states and the thermodynamic parameters extracted from these studies will contribute in governing the drug efficacy. Thus, understanding the protein-DNA interaction kinetics will greatly contribute to drug designing.

Mondal, Padmabati

Light-induced spin-crossover and single molecule magnetism in organometallic complex

Magnetic multi stability at the molecular level is at the origin of interesting potential application for information storage, quantum computing, molecular spintronic, magnetic sensors, switches and medical equipment. The most relevant type of material having the magnetic multi stability consists of molecules showing single molecule magnetism (SMM) and spin crossover (SCO) behaviors. In this project, theoretical and computational tools will be developed and employed to study the interplay of SMM and light-induced SCO systematically for transition metal-complex with the aim of exploring each and every key factors leading to the design principles of light-induced SMM and magnetic photo switch. The overall project is split into three quantum mechanical studies with increasing level of difficulty.

- Light-induced spin-crossover for Fe(II) complex.
- Single molecular magnetism of the Fe(II) complex.
- The light-induced SMM i.e. the interplay of light induced SCO and SMM.

The proposed project will have immense implications towards systematic understanding of electronic structure, properties and dynamics of light-induced SMM which will lead to better design of light-induced SMM for future application to molecular spintronics, quantum computing technologies.

Ramabhadran, Raghunath

Computational Astrochemistry: Probing the Evolution of Molecular Complexity in the Interstellar Medium

Molecular spectroscopy and computational chemistry play a decisive role to study astrochemical reactions.[1,2] On one side, astronomical observations of spectroscopic signatures provide the explicit proof of the presence of chemical species; on the other side, quantum chemistry allows shedding light on their formation/transformation mechanisms, which are nowadays still object of debate and often not experimentally investigable.

As part of our work on interstellar chemistry, we shall work on the following specific projects:

(i) Possible Mechanisms for the formation of Interstellar Propylene oxide: Propylene oxide is one of the smallest chiral molecules recently discovered in the ISM.[3] Its formation mechanisms could lead to possible routes for the origin of chirality. By using electronic structure calculations, and rate constant computations, we propose to study the various pathways via which propylene oxide could have formed in the ISM.

(ii) The interesting case of some missing molecules in the ISM: It is surprising to note that within any functional group series, some members are present but others are not (eg. CH_4 has been detected, but C_2H_6 has not been; whereas related CH_3SH, and CH_3OH have been). We shall probe the interesting absence of some of these missing molecules, which has not at all been studied so far.

(iii) Cluster models for modelling interstellar surface reactivity: Interstellar reactions are postulated to have occurred in either the gas-phase, or as surface reactions on interstellar ices. We shall use cluster models (not employed thus far) to mimic the interstellar surface chemistry.

Collaborate with experimental groups (in particular Dr. Sunil Kumar's group) to complement our theoretical/computational findings is also planned.

Sunil Kumar, S.

- Physics of the Interstellar Medium (ISM) & Atmospheric Sciences
    - Experimentally measure the rates of formation and destruction of molecules in interstellar conditions and earth's atmosphere
    - Data for modeling the ISM, earth's atmosphere, and cold plasma
- Origin of chirality in biomolecules
    - Biomolecules are either left-handed or right-handed
    - Probe the formation mechanisms of biomolecules in space
    - Polarization-dependent fluorescence spectroscopy

- Nature's choice of the molecules for building life
    - Measure the intrinsic photostability of biomolecules
    - Identify the effects of solvation on the structure and hence the function of biomolecules
- Theoretical evaluation of the rate coefficients to complement the experimental results.
- Theoretical evaluation of the structure of biomolecules in determining its intrinsic properties and their response to solvent environment.

Sharma, Arijit

Development of hybrid quantum networks

The development of quantum networks based on interlinked quantum nodes and secure

quantum communication channels are a major challenge in the field of quantum information science, including quantum communication, computing, and metrology. The development of hybrid quantum networks has been a new pathway that aims to combine the best of both of both worlds: fast read-out from quantum bits comprised of atoms and storage of quantum information in solid state counterparts like vacancy centers in Silicon or diamond. Hybrid quantum networks may provide opportunities and challenges across a range of technical frontiers including quantum computation, communication and metrology. Such networks might enable perfectly secure data transmission and enhanced data processing via distributed quantum computing. NV (nitrogen vacancy) centers in diamonds or color centers in silicon (Si) can be very promising candidates to ensure desired performance and fidelity both acting as a qubit for quantum computation and information processing and also as an interface to photons and thus operating as a quantum processor in quantum communication schemes. Our initial scientific objectives under CAMOST Phase-I proposal are as follows:

- Single photon generation from an atomic/solid state platform
- Demonstration of quantum entanglement and quantum network in the hybrid system
- Demonstration of quantum information processing schemes in the hybrid system

RECENT PUBLICATIONS of CORE Members of CAMOST

1. A. Sharma et. al, “Sawtooth-wave adiabatic-passage slowing of dysprosium”, Phys. Rev. A, Volume 99, PP 063414, June 2019.
2. A. Sharma et al.,”Optical control of resonant light transmission for an atom-cavity system”, Phys. Rev. A, Volume 91, PP 043824, Apr 2015.
3. A. Sharma et al., “Nonequilibrium Quantum Magnetism in a Dipolar Lattice Gas”, Phys. Rev. Lett., Volume 111, PP 185305, Oct 2013.
4. A. Sharma et al., “Cooling and stabilization by collisions in a mixed ion–atom system”, Nature Communications, Volume3, PP 1126, Oct 2012.
5. A. Sharma et al., “Probing spin dynamics from the Mott insulating to the superfluid regime in a dipolar lattice gas”, Phys. Rev. A, Volume 93, PP. 021603(R), Feb 2016
6. P. C. Deshmukh et al., “Wigner-Eisenbud-Smith photoionization time delay due to autoioinization resonances”, J. Phys. B: Atomic, Molecular and Optical Physics, Volume 51, PP. 065008, March (2018).
7. P. C. Deshmukh et al., “Strong dependence of photoionization time delay on energy and angle in the neighborhood of Fano resonances”, Phys. Rev. A, Volume 99, PP 013416, Jan 2019.
8. P. C. Deshmukh et al., “Wigner time delay in photodetachment”, Phys. Rev. A, Volume 99, PP 043407, Apr 2019.
9. P. C. Deshmukh et al., “Dominance of correlation and relativistic effects on photodetachment time delay well above threshold”, Phys. Rev. A, Volume 99, PP 063413, June 2019.
10. P. C. Deshmukh et al., “An Analytic Study of the Wiedemann-Franz Law and the Thermoelectric Figure of Merit”, Journal of Physics Communications, Volume 3, PP 105001, Oct 2019.
11. P. Mondal et al., “Impact of the redox state of flavin chromophores on the UV–vis spectra, redox and acidity constants and electron affinities”, J. Photochem. Photobiol. A: Chemistry, Volume 387, PP. 112164, October 2019.
12. P. Mondal and M. Huix-Rotllant, “Theoretical insights into the formation and stability of radical oxygen species in cryptochromes”, Phys. Chem. Chem. Phys., Volume 21, PP. 8874-8882, April 2019.
13. P. Mondal et al., “Azobenzene as a photoregulator covalently attached to RNA: a quantum mechanics/molecular mechanics-surface hopping dynamics study”, Chem. Sci., Volume 9, PP. 4671-4681, April 2018.
14. P. Mondal et al., “Ab initio study of dynamical E × e Jahn-Teller and spin-orbit coupling effects in the transition-metal trifluorides TiF_3, CrF_3, and NiF_3”, J. Chem. Phys., Volume 136, PP. 084308, January 2012.
15. Raghunath O. Ramabhadran et al., Weak Interactions in Interstellar Chemistry: How Do Open Shell Molecules Interact with Closed Shell Molecules?, ACS Earth Space Chem., Volume 3, PP. 1080-1095, April 2019.

16. Raghunath O. Ramabhadran et al., "How an early or late transition state impacts the stereoselectivity of tetrahydropyran formation by intramolecular oxa-Michael addition", Org. Biomol. Chem., Volume **17**, PP. 6293-6304, June 2019.

17. Raghunath O. Ramabhadran et al., "Mechanistic Insights of Cu(II)-Mediated ortho-C–H Amination of Arenes by Capturing Fleeting Intermediates and Theoretical Calculations", Chem. Commun., Volume 55, PP. 9359-9362, July 2019

18. Raghunath O. Ramabhadran et al., "Metal-Ion- and Hydrogen-Bond-Mediated Interstellar Prebiotic Chemistry: The First Step in the Formose Reaction", J. Phys. Chem. A, Volume 121, PP. 8659-8674, October 2017.

19. R. K. Gangwar, et al, "Autoresonance Cooling of Ions in an Electrostatic Ion Beam Trap", Physical Review Letters, Volume 119, PP103202, Sept 2017.

20. R. K. Gangwar, et al., "Modeling of laser produced Zn plasma with detailed electron impact fine structure excitation cross-sections, Plasma Sources Sci. Technol., Volume 28, PP 095009, Sept 2019.

21. R. K. Gangwar, et al, Nanoparticle synthesis by high-density plasma sustained in liquid organosilicon precursors, Journal of Applied Physics, Volume 122, PP 243301, Dec 2017.

22. R. K. Gangwar, et al., "Spectroscopic diagnostic of low pressure inductively coupled Kr plasma using a collisional radiative model with fully relativistic cross sections, Plasma Sources Science & Technology, Volume 25, PP 035025, May 2016.

23. R. K. Gangwar, et al, "Determination of the electron temperature in plane-to-plane He dielectric barrier discharges at atmospheric pressure", Plasma Sources Sci. Technol. Volume 25, PP 015011, Dec 2015.

24. Sunil Kumar et al., "Low temperature rates for key steps of interstellar gas-phase water formation", Sci. Advances, Volume 4, eaar3417, Jun 2018.

25. Sunil Kumar et al., "Photofragmentation mechanisms in protonated chiral cinchona alkaloids", Phys. Chem. Chem. Phys., Volume 18, PP. 22668 - 22677, July 2016.

26. Sunil Kumar et al., "Photodetachment as a destruction mechanism for CN– and C3N– anions in circumstellar envelopes", ApJ, Volume 776, September 2013.

27. Sunil Kumar et al., "UV photodissociation dynamics of deprotonated 2'-deoxyadenosine 5'-monophosphate $[5'\text{-dAMP-H}]^-$ ", J. Phys. Chem. A, Volume 115, PP.10383-10390, July 2011.

28. S. S. Mandal et al., "Nanomechanics of the substrate binding domain of Hsp70 determine its allosteric ATP-induced conformational change", Proc. Natl. Acad. Sci. U S A., Volume 114, PP. 6040-6045, June 2017.

29. S. S. Mandal et al., "Knotting and Unknotting of a Protein in Single Molecule Experiments", Proc. Natl. Acad. Sci. U S A., Volume 113, PP. 7533-7538, July 2016.

30. V P Majety et. al., "Evidence of Extreme Ultraviolet Superfluorescence in Xenon" Physical review letters, Volume 123, PP 023201, July 2019.

31. V P Majety et. al., Physical Review A, "Multielectron effects in strong-field ionization of CO_2: Impact on differential photoelectron spectra", Volume 96 , PP 053421, Nov 2017.

32. V P Majety et. al., “Dynamic Exchange in the Strong Field Ionization of Molecules” Physical Review Letters, Volume 115, PP 103002, Sept 2015.

33. V P Majety et. al., “Anomalous Fano Profiles in External Fields”, Physical review letters, Volume 115, PP 243001, Dec 2015.

34. V P Majety et. al., “Photoionization of few electron systems: a hybrid coupled channels approach”, New Journal of Physics, Volume 17, PP 063002, June 2015.