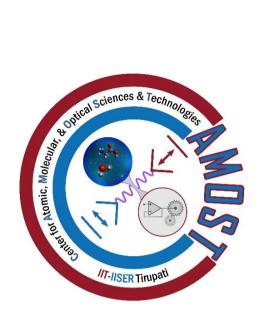
CAMOST Annual Report: 2021 - 2022



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

A JOINT INITIATIVE OF IIT TIRUPATI & IISER TIRUPATI







JOINT INITIATIVE OF IIT 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, the evolution of our Universe, secure communication, etc.

Tirupati is the only town in India that 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 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 biosciences
- Fostering human resources to meet 21stcentury 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



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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**



Tokyo Institute of Technology



Bhanu Pratap Das S T Manson Georgia State University TIFR, Mumbai



G Ravindrakumar



Roland Wester University of Innsbruck



Jan Michael Rost MPI for Complex Systems

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Core Administrative Members



Arijit Sharma Coordinator, IIT Tirupati



S Sunil Kumar Coordinator, IISER Tirupati



Reetesh Gangwar HoD, Physics, IIT Tirupati



G Ambika Chair, Physics, IISER Tirupati

Principal Investigators

IIT Tirupati



Arijit Sharma



Arun K Manna



Debasish Mondal



N N Murthy



P C Deshmukh



Rajib Biswas







Reetesh Gangwar

Swapnil Bhuktare Vijaya K Gurugubell Vinay P Majety Mamilla Ravi Sankar

Aravinda S

IISER Tirupati



Patmabati Mondal



Raghunath O R



Soumit Mandal



S Sunil Kumar



Sudipta Datta



Tapan C Adhyapak



Sasmita Mohakud



Rakesh S Singh



Ravi Kumar Pujala

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Adjunct Members



Dhananjay Nandi IISER Kolkata



G Aravind
IIT Madras



Koushik Saha IIT Dharwad



R Hari Varma IIT Mandi



Jobin Jose IIT Patna



Rajesh K Kushawaha PRL, Ahmedabad



S Sivakumar KREA University



Sivarama Krishnan IIT Madras



Ramachandra R Yalla University of Hyderabad



Sankar De SINP, Kolkata



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Events hosted by CAMOST (August 2021 – June 2022)

A comprehensive overview of CAMOST and its activities is available on the twin websites:

https://iittp.ac.in/camost

http://www.iisertirupati.ac.in/camost.

In addition to building up several collaborations among its members, CAMOST has organized several events such as seminars and plans to organize some additional events to commemorate its second year of operation.

First Anniversary Colloquium Series:

To commemorate the nucleation of CAMOST, we conducted CAMOST ANNIVERSARY WEEK COLLOQUIUM SERIES (16-20 August 2021). Five eminent scientists working on Quantum Science and Technologies and Plasma Science delivered lectures at this event.

Speaker	Affiliation	Date	Title of the talk	
Prof. G. Ravindrakumar	TIFR Mumbai	16.08.2021	Physics of extreme states created by tabletop lasers	
Prof. R. Vijayaraghavan	TIFR Mumbai	17.08.2021	How to build a quantum computer?	
Prof. Urbasi Sinha	RRI Bangalore	18.08.2021	Photonic quantum science and technologies	
Prof. Dmitry Budker	JGU Germany & UC Berkeley	19.08.2021	The perfect defect: Physics and sensing applications of the NV centers in diamond	
Prof. Peter Bruggeman	University of Minnesota	20.08.2021	Low-temperature plasma – A perspective	

Talks organized:

CAMOST organized two online webinars in the last year (August 2021 - June 2022).

- Dr. Sudipta Dutta, IISER Tirupati delivered a talk on "Tunable magnetic states in two-dimensional materials", 29 October 2021.
- Dr. Reetesh Kumar Gangwar, IIT Tirupati delivered a talk on "Spectroscopic diagnostic of argon rotating gliding discharges", 17 November 2021.

Special Issue of AAMOS20 proceedings in Physica Scripta:

CAMOST, along with Dayanand Sagar University, Bengaluru, co-hosted the international web conference: 'Advances in Atomic, Molecular, and Optical Sciences – 2020' (AAMOS20) from 14th to 18th December 2020. The conference was convened by an international committee of distinguished scientists from Australia, Japan, India, Ireland, and the USA. 37 talks over five days were delivered at AAMOS20 by leading experts from many countries which include Australia, Japan, China, India, Switzerland, Germany, Ireland, the UK, Italy, and the USA. The proceedings of AAMOS20 are being published by the Institute of Physics (UK) Journal Physica Scripta as a special focus issue. The details are available at the linked text below:

Advances in Atomic, Molecular, and Optical Sciences (2020) - Physica Scripta - IOPscience

Publications of CAMOST Members

In the past year (August 2021 – June 2022), CAMOST members have published 25 peer-reviewed journal articles in renowned international journals and two chapters in books.



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Journal Publications:

- 1. R. Ravindranath, **P. Mondal**, N. Gillet, Radical cation transfer in a guanine pair: An insight to the G-quadruplex structure role using constrained DFT/MM, Theo. Chem. Acc., **140**, 1 (2021)
- 2. **P. Mondal**, P. A. Cazade, A. K. Das, T. Bereau, M. Meuwly, *Multipolar Force Fields for Amide-I Spectroscopy from Conformational Dynamics of the Alanine Trimer*, J. Phys. Chem. B, **125**, 10928 (2021)
- 3. G. K, A. R. Thomas, T. S. Vyjayanthi, and **S. S. Mandal**, Structural and Thermodynamic Insights into the Cren7 Mediated DNA Organization in Crenarchaeota, Phys. Chem. Chem. Phys. (2022)
- 4. Km Akanksha Dubey and **Jobin Jose**, Elastic electron scattering from Ar@C60+: Dirac-partial wave analysis, J. Phys. B: At. Mol. Opt. Phys. **54**, 115204 (2021)
- 5. R. Rafeek and **D. Mondal**, Noise-induced symmetry breaking of self-regulators: An asymmetric transition towards homochirality, J. Chem. Phys., **154**, 244906 (2021)
- 6. T. Debnath, P. Chaudhury, T. Mukherjee, **D. Mondal**, and P. K. Ghosh, *Escape Kinetics of Self-Propelled Particles from a Circular Cavity*, J. Chem. Phys. **155**, 194102 (2021)
- 7. Subhasish Saha and **Jobin Jose**, Sensitivity of correlation effects and Shannon entropy in Be@C60 to the nature of confinement potentials, Phys. Scr. **96**, 094012 (2021)
- 8. Afsal Thuppilakkadan, **Jobin Jose**, and **Hari R Varma**, *Photoionization dynamics of Ar trapped in a fullerene anion: Coulomb confinement resonances in 2s subshell and its impact on the 3s subshell*, Phys. Scr. **96** 104004 (2021)
- 9. Km. Akanksha Dubey and **Jobin Jose**, Effect of charge transfer on elastic scattering of electron from Ar@C60: Dirac partial wave calculation, Eur. Phys. J. Plus **136**, 713 (2021)
- 10. Afsal Thuppilakkadan, **Jobin Jose**, and **Hari Varma**, *Confinement enhanced spin-orbit interchannel coupling effect on the atomic photoionization*, J. Phys. B: At. Mol. Opt. Phys **54**, 145001 (2021)
- 11. S. Adhikary, S. Mohakud, and **S. Dutta**, Engineering Anisotropic Klein Tunneling in Black Phosphorene through Elemental Substitution, Phys. Status Solidi B Basic Res. **258**, 2100071 (2021)
- 12. Hemanth Dinesan and **S. Sunil Kumar**, Laser-Induced Fluorescence (LIF) Spectroscopy of Trapped Molecular Ions in the Gas Phase, Applied Spectroscopy (2022, In press)
- 13. S. Y. Ali, R. Rafeek, and **D. Mondal**, Geometric Brownian Information Engine: Upper Bound of the Achievable Work under Feedback Control, J. Chem. Phys. **156**, 014902 (2022)
- 14. Vinay H. N.; K. P. Biligiri; M. Jagadeesh; **D. Mondal**, Development of Organoclay Suitable for Applications in Recycled Rubber-based Asphalt Binders: Montmorillonite Tailored with Quaternary Ammonium Salt, J. Mat. Civil Eng. (2022, In press)
- 15. Shaik Mahamad Allabakshi, P.S.N.S.R. Srikar, **R. K. Gangwar**, and S. M. Maliyekkal, *Feasibility of surface dielectric barrier discharge in wastewater treatment: Spectroscopic modeling, diagnostic, and dye mineralization*, Separation and Purification Technology (2022, In press)
- 16. S. S. Baghel, N. Sahin, A. Agrawal, **R. K. Gangwar**, M Tanı, sl, and R. Srivastava, *Diagnostic study* of capacitively coupled neon rf plasma with traces of O_2/H_2 at intermediate pressure, Journal of Physics D: Applied Physics, **55**, 295201 (2022)
- 17. Shruti Saraswat, Aiswarya R, and **Jobin Jose**, Shannon entropy of resonant scattered state in the $e-C_{60}$ elastic collision, J. Phys. B: At. Mol. Opt. Phys **55**, 055003 (2022)
- N. M. Hosea, J. Jose, and H. R. Varma, Near-threshold Cooper minimum in the photoionisation of the 2p subshell of sodium atom and its impact on the angular distribution parameter, J. Phys. B. At. Mol. Opt. Phys, 55, 135001 (2022)
- 19. Saha, S., Banerjee, S. & **Jose, J.** Impact of Charge Migration and the Angle-Resolved Photoionization Time Delays of the Free and Confined Atom X@C60. Atoms Peace Int. J. **10**, 44 (2022)
- 20. S. Baral, S. Saha, K. A. Dubey, **J. Jose**, **P. C. Deshmukh**, A. K. Razavi, and S. T. Manson, *Unusual behavior of Cooper minima of ns subshells in high-Z atoms*, Phys. Rev. A **105**, 062819 (2022)
- 21. S. S. Baghel, **R. K. Gangwar,** & R. Srivastava, Diagnostics of Ne Ar mixture plasma using a fine-structure resolved collisional radiative model. Contrib. Plasma Phys. **62**, (2022).
- 22. **Deshmukh, P. C.,** Ghosh, S., Kumar, U., Hareesh, C. & Aravind, G. A. *Primer on Path Integrals, Aharonov–Bohm Effect and the Geometric Phase.* The Phys. Educat. **04**, 2250005 (2022)



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- 23. S. Mondal, S. R. Das, L. Sahoo, **S. Dutta**, and U. K. Gautam, *Light-Induced Hypoxia in Carbon Quantum Dots and Ultrahigh Photocatalytic Efficiency*, J. Am. Chem. Soc. 144, 2580 (2022)
- 24. S. Karmakar and **S. Dutta**, Strain-Tuneable Photocatalytic Ability of BC₆N Monolayer: A First Principle Study, Comput. Mater. Sci. **202**, 111002 (2022)
- 25. M. K. Yadav, S. No. Sangitra, N. Panwar, T. Rimza, **R. K. Pujala**, and P. Kumar, *Aspect ratio dependent viscoelastic properties of graphene oxide liquid crystals*, Materials Chemistry and Physics, **287**, 126305 (2022)

Book Chapter/ Monographs:

- 1. A. Harafan, **R. K. Gangwar**, & S. M. Maliyekkal, Chapter 8 Abatement of pesticides in drinking water by nanoscale carbon materials. in Separation Science and Technology (ed. Ahuja, S.) vol. 15 139–161 (Academic Press, 2022).
- S. M. Allabakshi, P. S. N. S. Srikar, R.K. Gangwar, & S. M. Maliyekkal, Application of Plasma-Assisted Advanced Oxidation Processes for Removal of Emerging Contaminants in Water. in New Trends in Emerging Environmental Contaminants (eds. P. Singh, S., Agarwal, A. K., Gupta, T. & Maliyekkal, S. M.) 333–370 (Springer Singapore, 2022).

Invited lectures/talks/posters by CAMOST Members

In the past year (August 2021 – June 2022), several CAMOST members have been invited for seminars, talks, and poster presentations at several national and international conferences and workshops. The details are listed below:

Lectures/Talks:

- Debashis Mondal, Seminar: National and International Research Fellowships and Employment opportunities at Students' Week Celebrations event at Ramakrishna Mission Sikhshanamandira, Kolkata, India on 5 January 2022.
- 2. S. Sunil Kumar, Seminar: A story of mysterious molecules in space diffuse interstellar bands, Annual Research Conference organized from 21-25 February 2022 at Mahatma Gandhi College Thiruvananthapuram on 25 February 2022.
- 3. Arijit Sharma, Seminar: Towards developing the next generation portable atomic sensors based on the two-photon transition in warm atomic vapors for quantum communication, sensing, and positioning applications, at Indo-Israel Joint Workshop on Quantum Technologies organized jointly by DIA-CoE DRDO and IIT Delhi from 5-6 April 2022 at IIT Delhi on 6 April 2022.
- 4. Arijit Sharma, Seminar: Towards developing the next generation portable atomic sensors based on the two-photon transition in warm atomic vapors for quantum communication, sensing, and positioning applications, at TAMIONS II Conference and Discussion Meeting organized by ICTS Bengaluru from 9-13 May 2022 at ICTS Bengaluru on 11 May 2022.
- 5. Soumit Sankar Mondal, Seminar: *Protein dynamics at bulk and single molecule level*, 1 June 2022 at Guwahati University.
- Padmabati Mondal, Seminar: Pkay Development of a user-friendly and black-box method for reliable pka prediction, online conference organized from 11-14 December 2021 by IISER Kolkata/SNBNCBS/Kalyani University on 14 December 2021.
- Padmabati Mondal, Seminar: In Silico Decryption of Protein-Ligand Interaction, online conference organized from 11-14 December 2021 by IISER Kolkata/SNBNCBS/Kalyani University on 14 December 2021.
- 8. Ravi Kumar Pujala, Invited Talk in "Mathematics and Physics of Fluids 2021" jointly organized by the Disciplines of Mathematics and Physics, IIT Gandhinagar, during November 1-3, 2021.
- 9. Aravinda S, Introducing quantum computation using IBM qiskit IIT Kanpur, 7th and 12th April, 2022.
- 10. Aravinda S, On Quantum information theory and computation, Public talk at Cre'active' forum, Karnataka, March 19, 2022.



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- 11. Aravinda S, On the maximally entangled and entangling unitary operators and its role in constructing a Quantum Ergodic Hierarchy, ICQIF (International conference on quantum information and foundation) -2022 Kolkata, February 18, 2022.
- 12. Aravinda S, 4. Many-body entangled state in quantum information theory Faculty Development Program sponsored by ATAL, Tripura central university, February 8, 2022.

Posters:

- Salvi Mohandas, Franziska Dahlmann, Eric Endres, Sunil Kumar, and Roland Wester, Gas-phase spectroscopic study of [dAMP-H]⁻ in a cryogenic 16-pole wire trap, Early Career Conference in Trapped Ions (ECCTI) 2022, Date: 26 June 2022 to 1 July 2022, Location: CERN, Switzerland
- 2. Abhijit Kundu, Sumit Achar, Rashtrapriya Kumar Kapri and Dr. Arijit Sharma, Poster: Progress towards a cold atom-ion quantum network, at TAMIONS II Conference and Discussion Meeting organized by ICTS Bengaluru from 9-13 May 2022 at ICTS Bengaluru on 9-11 May 2022.
- 3. C. Rasadi Munasinghe, P. C. Deshmukh, S. T. Manson, Photoionization Branching Ratios of Spin-Orbit Doublets in Rn Far Above Thresholds, APS Division of Atomic, Molecular and Optical Physics (DAMOP), May 30 June 3, 2022, Orlando, Florida, USA
- 4. Aarthi Ganesan, Sourav Banerjee, Ankur Mandal, P. C. Deshmukh, S. T. Manson, Photoionization time delay of Hg 6s subshell at higher energies: RMCTD calculations, APS Division of Atomic, Molecular and Optical Physics (DAMOP), May 30 June 3, 2022, Orlando, Florida, USA
- 5. Rezvan Hussaini, P. C. Deshmukh, S. T. Manson, Angular Dependence of the Transition from Dipole to Quadrupole Photoionization Time Delay in Atoms, APS Division of Atomic, Molecular and Optical Physics (DAMOP), May 30 June 3, 2022, Orlando, Florida, USA
- 6. Soumyashree Baral, Jobin Jose, P. C. Deshmukh, S. T. Manson, 6p Cooper minima in the photoionization in high-Z atoms, APS Division of Atomic, Molecular and Optical Physics (DAMOP), May 30 June 3, 2022, Orlando, Florida, USA
- 7. Pratiksha Parajuli, P. C. Deshmukh, S. T. Manson, Nondipole Time Delay in the Photoionization of Atomic Systems, APS Division of Atomic, Molecular and Optical Physics (DAMOP), May 30 June 3, 2022, Orlando, Florida, USA
- 8. Nishita M Hosea, Jobin Jose, Hari Varma, P. C. Deshmukh, S. T. Manson, Photoionization dynamics of Na 3s in the Cooper minimum region, APS Division of Atomic, Molecular and Optical Physics (DAMOP), May 30 June 3, 2022, Orlando, Florida, USA
- 9. S. R. Valluri, Jisrawi Najeh, P. C. Deshmukh, Prabhat Reddy, Sibibalan, Solar Cells and the Lambert W Function, Canadian Association of Physics (CAP) Congress, June 5-10, 2022, McMaster University, Hamilton, Canada
- Jisrawi, Najeh; Valluri, S. R., P. C. Deshmukh, Shreyas Suresh, J. Jeysitharam, Metamaterials and the Lambert W function, Canadian Association of Physics (CAP) Congress, June 5-10, 2022, McMaster University, Hamilton, Canada

Sponsored research grants secured by CAMOST Members

In the past year (August 2021 – June 2022), CAMOST members have secured 2 sponsored research grants from external funding agencies.

S. No.	Project Coordinators	Project Title	Funding agency	Project Period	Sanctioned fund (INR)
1	Arijit Sharma (PI)	Development of a deterministic single-photon source for quantum technology applications	I-HUB Quantum Technology Foundation, IISER Pune	01 Mar 2022 – 28 Feb 2024	25.20 lakhs
2	S. Sunil Kumar (PI, IISER-T), Arijit Sharma (Co-PI,	Towards the development of fluorophores of	DST-SERB	22 Mar 2022 –	76.09 lakhs (out of which



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	IITT), and Padmabati Mondal (Co-PI, IISER-T)	predictable fluorescence: A comprehensive investigation of fluorescence characteristics of fluorescein		21 Mar 2025	INR 24.36 lakhs for IITT)
3	Tapan Chandra Adhyapak (PI), Ravi Kumar Pujala (Co-PI)	Hydrodynamic simulations and experiments on dense suspensions and near- surface trapping of flagellated bacteria	DST-SERB	Mar 2022 – Feb 2025	42.00 lakhs
4	Aravinda S (Co- PI)	Meity project with TCG Crest	Amazon Web Services		Time slots for quantum computational simulations

Research infrastructure supported by CAMOST

In the past year (August 2021 – June 2022), CAMOST has supported the procurement of the following equipment under research infrastructure support extended to CAMOST projects:

At IIT Tirupati:

- (i) DSO 4-Channel, 100MHz with sample rate 2 GS/s
- (ii) Arbitrary wave function generator Dual- channel, 25 MHz with sampling rate 125 MS/s
- (iii) 375 laser system for Ca ionization
- (iv) 422 laser system for Ca ionization
- (v) 850 laser system for Ca ion laser repumping
- (vi) 854 laser system for Ca ion laser repumping
- (vii) 866 laser system for Ca ion laser repumping
- (viii) 397 laser system for Ca ion laser cooling
- (ix) 780 laser system for Rb atom cooling
- (x) 780 laser system for Rb atom cooling
- (xi) Analog electronics module for reference cavity
- (xii) Kimball Physics two 16 port vacuum chambers made of SS 316L (non-magnetic steel) for Rb atom trap and Ca ion trap experiment
- (xiii) Laser wavelength meter with 10 MHz accuracy
- (xiv) RF Spectrum Analyzer 10kHz-9GHz
- (xv) Vacuum components (CF blanks, CF and KF bellows, CF conical nipples, CF I-piece, CF T-piece, CF 4-way cross) for the Rb atom experiment and the Ca ion trap experiment
- (xvi) Active Vibration Isolation Optical tables (10 feet X 4 feet) 2 nos.
- (xvii) Oscilloscopes 70 MHz 4 channel 2 Nos
- (xviii) Arbitrary wave function generators 2 Channel DC 20 MHz 3 nos
- (xix) Low ripple and low distortion programmable bipolar DC power supplies (0-30V, 0-5A) 3 numbers
- (xx) Data acquisition systems 200 MHz DSO (Digital Storage Oscilloscope)

At IISER Tirupati:

(i) Fast low noise high voltage switch Type – HS200 Dual