Annual Report 2020-2021 Center for Atomic, Molecular, and Optical Sciences & Technologies (CAMOST)

The Center for Atomic, Molecular, and Optical Sciences & Technologies (CAMOST) is a joint venture between IIT Tirupati and IISER Tirupati that has been established on 14th August 2020 to address key challenges in the frontier areas of AMO science and technology. The center aims to facilitate exchange of information, collaboration, and cross-fertilization of ideas relevant to the frontier areas of AMO science and technologies by allowing researchers from institutions pan-India to communicate and collaborate with each other under the aegis of CAMOST.

The center consists of a dedicated group of young scientists from IIT Tirupati and IISER Tirupati along with adjunct members from several other institutions of national importance. The following are the current thrust areas of the center:

- 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

Professor P C Deshmukh, IIT Tirupati, serves as the mentor and the convener of CAMOST. The administrative council consists of Professor K N Satyanarayana, the Director of IIT Tirupati and Professor K N Ganesh, the Director of IISER Tirupati. The scientific advisory committee is constituted by distinguished AMO scientists from India (Dilip Angom (PRL, Ahmedabad), E Krishnakumar (RRI, Bangalore), C P Safvan (IUAC, New Delhi), G Ravindra Kumar (TIFR, Mumbai)) and abroad (Dmitry Budker (JGU Mainz & UCB), John Costello (Dublin City University), Bhanu Pratap Das (Tokyo Institute of Technology), S T Manson (Georgia State University), Roland Wester (University of Innsbruck), Jan Michael Rost (MPI for Complex Systems), and Professor Peter Bruggeman (University of Minnesota)).

Inauguration ceremony of CAMOST

The center was inaugurated by Dr. Arabinda Mitra, Secretary to the Office of the Principal Scientific Advisor (PSA) on 14th August 2020. Dr. Mitra released the CAMOST brochure and a short video providing a glimpse of the origins of CAMOST and the activities that the center will carry out. The inauguration event was attended by Directors of both the institutions, IIT Tirupati and IISER Tirupati, eminent and distinguished scientists in Atomic, Molecular and Optical Sciences from both India and abroad, and by several other participants including students and faculty from the two institutes.

Events hosted by CAMOST

A comprehensive overview of CAMOST and its activities are made available in the twin websites:

https://iittp.ac.in/camost

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

In addition to building up of several collaborations among its members, CAMOST has organized several events such as an international conference, seminars, and a minicourse on quantum optics.

International conference: Advances in Atomic, Molecular, and Optical Sciences – 2020 (AMOS2020)

The Center for Atomic, Molecular and Optical Sciences and Technology (CAMOST), IITT, along with Dayanand Sagar University, Bengaluru, co-hosted the international 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 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, UK, Italy, and USA. The proceedings of AAMOS20 are being published by the Institute of Physics (UK) Journal Physica Scripta as a special focus issue. The conference was streamed live on YouTube and is accessible at the link: https://www.youtube.com/c/IISERTirupatiofficial. A screenshot from the virtual conference is seen in figure below.



Talks organized:

CAMOST organized seminars four talks in the last year.

- Rajib Biswas, IIT Tirupati delivered a talk on "Theoretical Spectroscopy: From Proton Transfer to Hydrophobic Hydration", 15 October 2020.
- Sunil Kumar S, IISER Tirupati delivered a talk on "A novel experimental approach to probe the effect of environment on fluorescence properties of molecular ions", 19 November 2020.
- Padmabati Mondal, IISER Tirupati delivered a talk on "Photophysics and photochemistry of Indole and Indole derivatives: A quantum chemical study", 19 February 2021
- Anand Kumar Jha, IIT Kanpur delivered a talk on "Partial coherence: Applications in quantum state measurement, imaging and communication", 25 March 2021

Short online course on Quantum Optics:

CAMOST organized a short online course on Quantum Optics offered by Professor Sonjoy Majumder of Indian Institute of Technology Kharagpur from 19th July 2020 to 30th July 2020. It was a 10-day lecture series along with four tutorial sessions. It was a very-well received course attended by more than 200 participants. The lectures and tutorials were streamed live on YouTube, and it is available for reference at the link: https://www.youtube.com/c/IISERTirupatiofficial.

CAMOST Webinars:

CAMOST organized four webinars in the last year.

- 1. Dr Rajib Biswas, IIT Tirupati Title: Theoretical Spectroscopy: From Proton Transfer to Hydrophobic Hydration
- Dr S Sunil Kumar, IISER Tirupati
 Title: A novel experimental approach to probe the effect of environment on fluorescence properties of molecular ions
- Dr Padmabati Mondal, IISER Tirupati
 Title: Photophysics and photochemistry of Indole and Indole derivatives: A quantum chemical study
- 4. Dr. Ananad Kumar Jha, Department of Physics, Indian Institute of Technology Kanpur Title: Partial coherence: Applications in quantum state measurement, imaging, and communication

Publications of CAMOST Members

In the past year, CAMOST members have published 19 peer-reviewed journal articles in renowned international journals.

- Kambham Devendra Reddy and Rajib Biswas, <u>Theoretical spectroscopy of isotopically dilute water and</u> <u>hydrophobicity</u>, J. Chem. Phys. **153**, 094501, Sep 2020
- Salvi M, Raghunath Ozhapakkam Ramabhadran, and Sunil Kumar S, <u>Theoretical Investigation of a Vital</u> <u>Step in the Gasphase Formation of Interstellar Ammonia: NH₂⁺ + H₂ → NH₃⁺ + H, J. Phys. Chem. A 124, 8373, Sep 2020
 </u>
- Roshni W Pereira and Raghunath O Ramabhadran, <u>pK-Yay: A Black-Box Method using Density</u> <u>Functional Theory and Implicit Solvation Models to Compute Aqueous pKas of Weak and Strong Acids</u>, J. Phys. Chem. A **124**, 9061, Sep 2020

- Aarthi Ganesan, Sourav Banerjee, Pranawa C Deshmukh, and Steven T Manson, <u>Photoionization of Xe</u> <u>5s: angular distribution and Wigner time delay in the vicinity of the second Cooper minimum</u>, J. Phys. B: At. Molec. Opt. Phys. **53**, 225206, Oct 2020
- 5. Padmabati Mondal, <u>In silico decryption of serotonin–receptor binding: local non-covalent interactions</u> <u>and long-range conformational changes</u>, RSC Adv. **10**, 37995, Oct 2020
- Dipayan Chakraborty and Dhananjay Nandi, <u>Absolute dissociative electron attachment cross-section</u> <u>measurement of difluoromethane</u>, Phys. Rev. A **102**, 052801, Nov 2020
- 7. P C Deshmukh and Sourav Banerjee, <u>*Time delay in atomic and molecular collisions and photoionisation/photodetachment*</u>, Int. Rev. Phys. Chem. **40**, 127, Nov 2020
- 8. Souren Adhikary, Sudipta Dutta, and Sasmita Mohakud, <u>Antiferromagnetic spin ordering in two-</u> <u>dimensional honeycomb lattice of SiP</u>₃, Nanoscale Adv. **3**, 2217, Mar 2021
- R. Püttner, J. B. Martins, T. Marchenko, O. Travnikova, R. Guillemin, L. Journel, I. Ismail, G. Goldsztejn, D. Koulentianos, D. Ceolin, M. L. M. Rocco, M. N. Piancastelli, M. Simon, D. A. Keating, C. R. Munasinghe, P. C. Deshmukh, and S. T. Manson, *Nonstatistical behavior of the photoionization of spinorbit doublets*, J. Phys. B: At. Mol. Opt. Phys. **54**, 085001, May 2021
- Ankur Mandal, Pranawa C Deshmukh, and Kamal P Singh, <u>Controlling high harmonic generation using</u> <u>inhomogeneous two-color driving laser pulse</u>, Laser Physics **31**, 075302, May 2021
- 11. P C Deshmukh, J Jose, H R Varma, and S Manson, <u>Electronic structure and dynamics of confined atoms</u>, Eur. Phys. J. D **75**, 166, May 2021
- S. S. Baghel, S. Gupta, R. K. Gangwar, and R. Srivastava, <u>Diagnostics of Laser-Produced Mg Plasma</u> <u>through a Detailed Collisional Radiative Model with Reliable Electron Impact Fine Structure Excitation</u> <u>Cross-Sections and Self-Absorption Intensity Correction</u>, Plasma Sources Sci. Technol. **30**, 055010, May 2021
- 13. J. Ananthanarasimhan, R. K. Gangwar, P. Leelesh, P. S. N. S. R. Srikar, A. M. Shivapuji, and L. Rao, *Estimation of Electron Density and Temperature in an Argon Rotating Gliding Arc Using Optical and Electrical Measurements*, J. Appl. Phys. **129**, 223301, Jun 2021
- 14. Sourav Banerjee, G. Aarthi, Soumyajit Saha, Aravind Gopalan, P.C. Deshmukh, <u>*Time delay in negative</u>* <u>ion photodetachment</u>, Phys. Scr., **96**, 114005, Jul 2021</u>
- 15. Gayathry Rajeevan, Salvi Mohandas, and S Sunil Kumar, <u>Numerical simulations of storage and</u> <u>thermometry of small biomolecular ions in a 16-pole ion trap and a 16-wire ion trap</u>, Phys. Scr., 96, 124001, Aug 2021
- 16. P.C. Deshmukh, S. Banerjee, A. Mandal, and S. T. Manson, *<u>Eisenbud–Wigner–Smith time delay in</u> <u>atom–laser interactions</u>, Eur. Phys. J. Spec., 2021 (In press)*
- 17. P.C. Deshmukh, Aarthi Ganesan, Sourav Banerjee, and Ankur Mandal, <u>Accidental Degeneracy of the</u> <u>Hydrogen Atom and its Non-accidental Solution in Parabolic Coordinates</u>, Can. J. Phys., 2021 (In press)
- A. Maignan, L. Prabhat Reddy, S. Jeevanandam, P. C. Deshmukh, Ken Roberts, Najeh Jisrawi, and S. R. Valluri, <u>The electronic properties of graphene nanoribbons and the offset logarithm function</u>, Materials Today: Proceedings, 2021 (In press)
- D. Müll, F. Grussie, K. Blaum, S. George, J. Göck, M. Grieser, R. von Hahn, Z. Harman, Á. Kálosi, C. H. Keitel, C. Krantz, C. Lyu, O. Novotný, F. Nuesslein, D. Paul, V. C. Schmidt, S. Singh, S. Sunil Kumar, X. Urbain, A. Wolf, and H. Kreckel, <u>Metastable states of Si⁻ observed in a cryogenic storage ring</u>, Phys. Rev. A (In press, 2021)