

CURRICULUM VITAE



Dr. S.ATHIMOOLAM

Department of Physics
Anna University Regional Campus - Tirunelveli
Tirunelveli - 627 007
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Vidwan profile @: <https://ucen.irins.org/profile/235881>

Google Scholar @: <https://scholar.google.co.in/citations?hl=en&user=q-sM7awAAAAJ>

Scopus @: <https://www.scopus.com/authid/detail.uri?authorId=57203385769>

Educational Qualifications

Ph. D. in Physics (X-ray Crystallography)

School of Physics, MaduraiKamarajUniversity,
Madurai, Tamil Nadu. India

- Awarded on March 2008

M.Phil. in Physics

ManonmaniamSundaranarUniversity,
Tirunelveli, Tamil Nadu. India.

- Nov. 2004 - I Class

M.Sc.in Physics

Sri Paramakalyani College,
Alwarkurichi. Tamil Nadu. India.

- April 2003 - I Class

PGDCA(Post Graduate Diploma in Computer Applications)

AlagappaUniversity (Distance Education)
Karaikudi.

- July 2002 - I Class

B.Sc. in Physics

SriParamakalyaniCollege,
Alwarkurichi. Tamil Nadu. India.

- April 2001 - I Class

Ph.D. title - 'Crystal structure analyses of the complexes of some vitamins with some inorganic/organic acids'

Project in M.Phil. - 'Crystal and Molecular Structure analyses of Copper thiourea complex'

Project in M.Sc. - 'Growth of CaCO₃, BaCO₃ and ADP and their IR and XRD studies'

Proficiency on research -

- ␣ Structure solution of small molecules with single crystal X-ray diffraction and hydrogen bonding studies
- ␣ Growth of organic crystals with suitable methods especially pharmaceutical drugs and its salts, co-crystals and metal complexes
- ␣ Quantum chemical studies with Gaussian for optimization and vibrational analyses
- ␣ Vibrational and thermal spectral analyses
- ␣ Handled CAD4 Nonius MACH3 X-ray diffractometer instrument at School of Physics, Madurai Kamaraj University for more than three years in data collection and structure solutions.

Working Experience:

Teaching / Research (Full-time) experience:

<i>Position</i>	<i>Institute</i>	<i>Period</i>	<i>Experience</i>	
			Years	Months
AssistantProfessor in Physics	Anna University Regional Campus, Tirunelveli 627 007	From August, 2023 - till date	0	02
AssistantProfessor in Physics	UniversityCollege of Engineering, Anna University, Tirunelveli Region, Nagercoil 629 004	From September, 2009 - till date	14	0
Lecturer in Physics	Kalasalingam University, Anand nagar, Krishnan koil - 626 190.	From July, 2007 - September, 2009	2	02
Full-time Research scholar (DSTproject)	School of Physics, MaduraiKamarajUniversity, Madurai - 625 021. India.	From September 2004 - July, 2007	2	10
Lecturer in Physics	P.A.C.R.PolytechnicCollege, Rajapalayam, India.	From June 2003 - September 2004	1	04
Total			20	6

Research Interest

Crystal and molecular structure analyses, hydrogen bonding analyses, Coordination and inclusion compounds, phase transition studies, IR and Raman spectral analyses, DFT related theoretical studies, nano drug synthesis and characterization, etc.

Funded Research Projects executed:

S. No.	Title of the project	Name of the Funding agency	Period	Fund value (in lakhs)
1.	Synthesis, crystallization, characterization and molecular interactions on anticancer drugs: mercaptopurine, triethylenemelamine and their new complexes	DST - SERC (Young Scientist Programme)	August, 2012 - July, 2015	17.42

Research facilities developed at Dept. of Physics, UCEN [Molecular Structure Laboratory]:

- Ultrasonic Irradiator for preparation for nano drugs
- Constant Temperature Bath for bulk crystal growth
- Microwave Irradiator for synthesis of nano drugs for biological applications
- Digital balance with 0.001 gm accuracy
- Magnetic stirrer with hot plates for preparation of parent solution
- Cambridge Crystallographic Structural Database (CSD)
- Gaussian for molecular optimization and related studies
- WINGX and SHELXL-2014 for structure solving and refinement

Research Guidance & Scholar Details:

No.	Scholar details	Title / Area of research	Current status
Ph.D. Scholars			
8	Mr. T. Sterlin Raj [Reg. No. 1414789120]	Characterization studies of a fibrinolytic enzyme isolated from bacillus flexus for cardiovascular applications	Completed (2022)
7	Mrs. M. Mary Latha [Reg. No.1524789139]	Molecular investigations and vibrational analyses of some pharmacological compounds: theoretical and experimental approach	Completed (2021)

No.	Scholar details	Title / Area of research	Current status
6	Mr. L. Mary Novena [Reg. No.1524789137]	Structural and spectroscopic investigation of some drug crystals and its complexes using experimental and theoretical perspectives	Completed (2020)
5	Mr. S. Suresh Kumar [Reg. No. 1412789107]	Structural investigation on antineoplastic drugs and its complexes	Completed (2019)
4	Mrs. E. Arockia Jeya Yasmi Prabha [Reg. No. 1223789747]	Crystallization and characterization of pharmacologically important some heterocyclic compounds	Completed (2019)
3	S. Thangarasu (part-time scholar from KLU)	Structural Vibrational Thermal and Quantum Chemical Studies on Some 2-Aminopyrimidine and 3-Nitroaniline Complexes	Completed (2017)
2	A. Chitra devi (part-time scholar from KLU)	XRD, quantumchemical, vibrational spectra, thermal and biological studies on 4-aminoantipyrine salts	Completed (2016)
1	V. Susindran (part-time scholar from KLU)	Structural studies on some pyrazole derivatives and structure, vibrational, thermal and optical analyses of some anthralinic acid complexes	Completed (2015)
M.Phil. Scholars			
6	Mr. L Xavier Prince (under DDE, MKU, Madurai)	Theoretical and Experimental studies on structure and vibrational spectral analysis of nicotinamidium (a B-vitamin) hydrogen oxalate	Completed
5	Mr. M. Muthuraj (under DDE, MKU, Madurai)	Structural investigations on Vitamin L complex	Completed
4	Mrs. Navarani mala (under American College, Madurai; as a co-guide)	Spectroscopic investigations on hydrated 2-carboxyanilinium tartarate	Completed
3	Mrs. R. Sangeetha (under DDE, MKU, Madurai)	Crystal growth and spectral investigations on anthranilic acid complexes	Completed

No.	Scholar details	Title / Area of research	Current status
2	Mrs. N. Mahalakshmi Lavanya (under DDE, MSU, Tirunelveli)	Crystal and molecular structure of 2,3,6-Triphenylpiperidin-4-one	Completed
1	Mrs. V. Anu radha (under DDE, MKU, Madurai)	Crystal and molecular structure of 1'-Methyl-4'-(1-naphthyl)-3''-(1-naphthylmethylene)acenaphthene-1-spiro-2'-pyrrolidine-3'-spiro-1''-cyclohexane-2,2''-dione	Completed

Administrative responsibilities:

- ✓ **Head, Department of Science & Humanities** of Anna University Regional Campus, Tirunelveli from 26th September, 2023 to till date
- ✓ **Nodal Officer, Indian Research Information Network Systems (IRINS)** of Anna University Regional Campus, Tirunelveli from 9th August, 2023 to till date
- ✓ **Nodal Officer, Indian Research Information Network Systems (IRINS)** of University College of Engineering, Nagercoil from 26th October, 2021 to 2nd August, 2023
- ✓ **Zonal Officer, Zone XVII** of Anna University, Chennai from May, 2018 to 2nd August, 2023
- ✓ **First year coordinator**, UCEN from August, 2017 to December, 2019
- ✓ **Head, Department of Physics**, UCEN from 1st October, 2015 to December, 2019
- ✓ **Physics Lab In-Charge**, from 1st August, 2018 to 2nd August, 2023
- ✓ **Member Secretary**, College Council from June 2014 to October 2018
- ✓ **Secretary** for college canteen committee for three years, viz., 2013-14, 2014-15 & 2015-16
- ✓ **Executive Warden** for the UCEN College hostels from November, 2015 to May, 2018
- ✓ **Deputy Warden (Mess & Accounts)** for the UCEN hostels from November, 2012 to October, 2015
- ✓ **Zonal Officer, Zone XVII** of Anna University, Chennai from July, 2013 to March, 2014

- ✓ **Nodal Officer** for All India Survey on Higher Education (AISHE), Government of India from 2013-14 to 2017-18
- ✓ Discharged the duty as **convener for Government Free Laptop Scheme** 2012-13 & 2013-14
- ✓ **Camp Officer** for four central valuations of Anna University, Chennai at zone 17, UCEN [2011-12 (odd & even semesters), 2012-13 (odd & even semesters)]
- ✓ Acted as **Chief Superintendent for Anna University Examinations** for three semesters, viz., 2009-10 (even semester), 2010-2011 (odd & even semesters)
- ✓ Acted as **Course Coordinator** for the Engineering Physics I & II at Kalasalingam University for the academic year 2008-2009
- ✓ Acted as **Assistant Warden** for Hostels at Kalasalingam University from July 2007 to August 2008

Membership in registered society:

- ✓ On World Directory of Crystallographers (IUCr) - IUCr10806
- ✓ Life Member of Vignana Bharathi (VIBHA) - from 2023
- ✓ Member of Material Research Society of India (MRSI) - LMB2472
- ✓ Member of Indian Society of Atomic and Molecular Physics (ISAMP) - 1496
- ✓ Member of Indian Society for Technical Education (ISTE) - LM59056 yr. 2008
- ✓ Member of Indian Association of Physics Teachers (IAPT) - L4942

Members of academic/research related committees:

- ❖ Member of 83rd *Academic Council* of Sri Parasakthi College for Women (Under the Management of HR&CE Dept.), Courtallam 627 802 for the academic year 2022-23 (Meeting held on 14.09.2022)
- ❖ Member of 82nd *Academic Council* of Sri Parasakthi College for Women (Under the Management of HR&CE Dept.), Courtallam 627 802 for the academic year 2021-22 (Meeting held on 30.03.2022)
- ❖ Member of the Doctoral Committee for various scholars of Anna University and Manonmanian Sundaranar University

Books published:

- ❖ "Physics for Materials Science", M. Suresh & **S. Athimoolam**, Wakeup Publication, Chennai, Feb 2019, ISBN: 978-81-90856-768

- ❖ "Engineering Physics", M. Suresh & S. Athimoolam, Wakeup Publication, Chennai, July 2017, ISBN: 978-81-90856-728
- ❖ "Engineering Physics-II ", M. Suresh & S. Athimoolam, Wakeup Publication, Chennai, June 2015, ISBN: 978-81-90856-720.
- ❖ "Engineering Physics Laboratory Manual", M. Suresh & S. Athimoolam, Wakeup Publications, July 2015, ISBN: 978-81-90856-737.
- ❖ "Engineering Physics Laboratory Manual", M. Suresh & S. Athimoolam, Wakeup publications, Chennai, July 2015, ISBN: 978-81-90856-758.

List of workshops/FDP/skill development programmes attended:

20. Completed "AICTE Online Faculty Induction Training Programme for Technical Teachers (8 Module Courses)" for Faculty members organized by National Institute of Technical Teachers Training and Research (NITTTR) from April-May 2022.
19. Completed five days FDP on "Universal Human Values (UHV) in Education" organized by AICTE from 22.11.2021 to 26.11.2021.
18. Completed Two-Week (14 days) Interdisciplinary FDP on "Structural Analysis Using Rietveld Refinement, Microscopic and Compositional Analysis" organized by Guru Angad Dev Teaching Learning Centre, University of Delhi in collaboration with St. John's College, Agra, Bishop Moore College, Mavelikara, Catholicate College, Pathanamthitta, Sacred Heart College, Chalakudy and Christ College, Irinjalakudai under Pandit Madan Mohan Malaviya National Mission on Teachers and Training (PMMMNTT) from 29.09.2021 to 13.10.2021.
17. Completed six days FDP on "Recent Developments in Materials Science - 21" organized by Department of Physics and Chemistry, Sree Saraswathi Thyagaraja College, Pollachi, Coimbatore from 16.06.2021 to 22.06.2021.
16. Completed five days AICTE Training and Learning (ATAL) Academy online FDP on "Leadership & Excellence" organized by "PDPM Indian Institute of Information Technology, Design & Manufacturing, Jabalpur" from 07.09.2020 to 11.09.2020.
15. Completed three months (90 days) professional research training through "CSIR-Summer Research Training Program (SRTP-2020), CSIR-Indian Institute of Chemical Technology (CSIR-IICT)" with the mentor Dr. B. Sridhar, Principal Scientist, CSIR-Indian Institute of Chemical Technology, Hyderabad-500007, India from June, 2020 to August, 2020 and direct interaction with the scientist from 03.08.2020 to 31.08.2020 (29 days).
14. Completed 20 days "internship programme" in the 1st virtual summerschool on "Nanoscience and Nanomaterials" organized by the National Centre for Nanoscience and Nanotechnology, University of Madras from 10th July, 2020 to 30th July, 2020.

13. Participated in the **Science Academics' Science Leadership Workshop** (India's first science Leadership Program) organized by the Central University of Punjab, Bathinda during 22nd to 28th June, 2020.
12. Completed **Two-Week (14 days) FDP on "Managing online classes and co-creating MOOCs -FDPMOOCs02"** organized by Teaching Learning Centre & Research Development Service Cell, Ramanujan College, University of Delhi through Pandit Madan Mohan Malaviya National Mission on Teachers and Teaching (PMMMNTT), MHRD from 18th May, 2020 to 1st June, 2020.
11. Completed 10 days Indian **Summer School on Crystal Growth (ISSCG-2020)** - online mode Organized by SSN Research Centre, SSN Institutions (Autonomous), Chennai-603110, Tamil Nadu, Indian association with Indian Association for Crystal Growth (IACG) from 14th to 23rd May, 2020.
10. Completed **Two-Week (14 days) "Refresher Course in Human Rights"** conducted by UGC-Human Resource Development Centre, Bharathiar University, Coimbatore-641046 from 12.09.2019 to 25.09.2019.
9. Completed an **AICTE approved FDP (FDP101x) on "Foundation program in ICT for Education"** conducted by IIT, Bombay from 8th March, 2018 to 12th April, 2018 under the aegis of PMMMNTT, MHRD, GoI program.
8. Completed 16 days "**Science Academics' Refresher Course in Experimental Physics**" held at Thiagarajar College of Engineering, Madurai during 5th to 20th July, 2016
7. Completed three days "**Lecture Workshop on Materials Science and Engineering**" held at Thiagarajar College of Engineering, Madurai during March 9-11, 2016.
6. Completed the **two-week (14 days) ISTE short term training programme on "Engineering Physics"** conducted by IIT, Bombay from December 8 - 18, 2015 held under the National Mission on Education through ICT (MHRD).
5. Attended two days "**Bridge course on Physics**" conducted at Centre for Faculty Development, Anna University, Chennai 600 025 on 25th & 26th, June, 2014
4. Completed five days workshop on "**Introduction to Gaussian: Theory and Practice**" held at Delhi, India during 17th - 21st, December, 2012 organized by Gaussian, Inc.
3. Attended **International workshop on Crystal Growth and Characterization of Advanced Materials** during 9th to 13th January, 2006 at Crystal Growth Centre, Anna University, Chennai - 25
2. Attended **Annual Photonics Workshop 2005** during 26th to 28th February, 2005 at International School of Photonics, CUSAT, Kochi.
1. Completed **PLANEX workshop on Planetary Atmospheres, Ionospheres and Magnetospheres** during 17th to 22nd February, 2003 at Space Physics Laboratory, Vikram Sarabhai Space Centre, Thiruvananthapuram.

List of invited talks delivered in **International / national conferences / seminars / FDPs / webinars:**

27. "Influence of intermolecular interactions in Tailored molecular assembly" - Two Day National Seminar entitled "Recent Trends in Physical Sciences - RTPS 2023" during 02.02.2023 - 03.02.2023.
26. "Hands on training on structural elucidation of single crystals with online tools" - Two days workshop conducted by Kalasalingam Academy of Research and Education (KARE) on 24th and 25th July, 2020.
25. "Theoretical perceptive on the structure elucidation of single crystals" - Two days workshop conducted by Kalasalingam Academy of Research and Education (KARE) on 24th and 25th July, 2020.
24. "Classical and non-classical hydrogen bonds in compounds of Bronchodialator: Theophylline" - International Webinar series on "Advanced Materials for Sustainable Development" conducted by Kalasalingam Academy of Research and Education (KARE) on 2nd and 3rd July, 2020.
23. "Molecular Level investigation on Organic Materials" - a webinar conducted by Department of Nano Science and Nano technology, S.T. Hindu College, Nagercoil 629 002 on 29th May, 2020.
22. "Influence of Hydrogen Bonds in Nonlinear Optical Materials" - National level Faculty Development Programme (FDP) conducted by Kalasalingam Academy of Research and Education (KARE) on 26th May, 2020.
21. "Crystallography and its applications" - a live webinar conducted by Er. Perumal Manimekalai College of Engineering, Hosur 635 117 on 8th May, 2020 (1400 registered participants).
20. "Structural, spectroscopic and intermolecular interaction studies on a bronchodilator drug" - National Seminar on Technologically Important Crystalline and Amorphous Solids (TICAS-2019), Kalasalingam University, Krishnankoil, 5th& 6th April 2019.
19. "Experimental and theoretical perspectives of hydrogenbonded drug molecular crystals" - 23rd National Seminar on Crystal Growth and Applications (NSCGA-2019), held at Department of Physics, Bharathiar University, Coimbatore, Tamil Nadu- 641 046, on 28th - 30th January 2019.
18. "Laser Physics" - delivered invited talk at FDTP programme held at University College of Engineering - Dindigul, Anna University, Dindigul, on 25th June, 2018.
17. "Influence of hydrogen bonding metrics on nonlinear optical crystals" - 4th National Seminar on Technologically Important Crystalline and Amorphous Solids (TICAS-2018), Kalasalingam University, Krishnankoil, 2nd March & 3rd March, 2018.
16. "Hydrogen bonded assembly in nonlinear optical materials" - 22nd National Seminar on Crystal Growth and Applications (XXII NSCGA-2018) held at Department of Physics, Sacred Heart College (Autonomous), Tirupattur - 635601, on 29-31st

January 2018.

15. "*Hydrogen bonding interactions in anticancer drug molecules*" - International Seminar on Multidisciplinary Research in Chemistry, held at Department of Chemistry, Sri Saradha College for Women, Tirunelveli - 627011, on 6th September, 2017.
14. "*Crystallography and hydrogen bonds*" - delivered an invited talk at National Conference on Emerging Sensor Devices, Materials & Technologies (NCESDMT-2017) organized by our Department of Physics, Chikkanna Government Arts College, Tiruppur, Tamilnadu, India during 19th& 20th January, 2017.
13. "*Crystal growth and hydrogen bonds*" - delivered Guest Lecture at Sarah Tucker College, Tirunelveli on 4th January, 2017.
12. "*Current research on hydrogen bonds*" - delivered Guest Lecture at Womens' Christian College, Nagercoil on 23th August, 2016.
11. "*Crystallography and Intermolecular interactions*" - delivered at FDP programme on the title "Recent Advancements in Materials (FDP-RAM'16)" held at Bharathidasan Institute of Technology (BIT) campus, Anna University, Tiruchirappalli - 620024, 21st July, 2016.
10. "*Hydrogen bonding interactions in organic systems*" - delivered at "International Conference on Integration of STEM Education and Mental Health (ICISEM16), Special Session entitled: Advances in Applied Sciences" at Department of Physics, Noorul Islam centre for Higher Education (Noorul Islam University), Kumaracoil, Thucklay -629 180, 20th& 21st June, 2016
9. "*Materials Science and Engineering*" - delivered at Three day workshop on 'Physics in Engineering (PiE-II)' at Thiagarajar College of Engineering, Madurai, 9 - 11, March, 2016
8. "*Applications of Material Science*" - delivered Guest Lecture at M. Kumarasamy College of Engineering, Karur, 23rd& 24th February 2016
7. "*Hydrogen bond interactions in pharmacological compounds*" - Seminar on Recent Trends in Materials Science (RTMS), Department of Physics, Sadakathullah Appa College., Tirunelveli, 11th Jan 2016
6. "*Crystallography and Density Functional Theory*" - Two weeks FDP on Advanced Research in Materials for Engineering & Technological Applications (ARMETA-2015) at Bharathidasan Institute of Technology (BIT) campus, Anna University, Tiruchirappalli - 24 during 17th - 30th July, 2015
5. Delivered invited talk on 11.06.2015 in the Faculty Development programme on "*Changing Scenario in Materials Research*" organized by Department of Physics, Kalasalingam University, Krishnan koil during 8th - 12th, June, 2015
4. Delivered invited talk on 10.06.2015 in the Faculty Development programme on "*Changing Scenario in Materials Research*" organized by Department of Physics, Kalasalingam University, Krishnan koil during 8th - 12th, June, 2015
3. "*Hydrogen bonds in intermolecular assembly of vitamin crystals*" - International conference on Recent trends in Materials - 2014, organized by Department of

- Physics, Devanga Arts College, Aruppukkotai during 22nd& 23rdDecember-2014.
2. "*Hydrogen bonding investigations on biologically important molecules: a search for supramolecular assembly*" - National Seminar on Technologically Important Crystalline and Amorphous Solids (TICAS-2014), Kalasalingam University, Krishnankoil, 28th February & 1st March 2014.
 1. "*Hydrogen bonding investigations on organic molecules: a search for supramolecular assembly*" - National Seminar on Technologically Important Crystalline and Amorphous Solids (TICAS-2013), Kalasalingam University, Krishnankoil, 1st& 2nd, March - 2013.

Seminars / conferences / events organised/delivered lecture for popularization of science to the society conducted / contributed:

- 25 Delivered a Guest Lecture in the title of "*Simply be a Physicist*", at Department of Physics, Kalasalingam Academy of Research and Education (KARE), Krishnankoil on 30th September 2023.
- 24 Delivered a Invited talk in the title of "*Innovations lead the mankind*" at University College of Engineering, Thirukkuvalai at Induction Programme of First Year Fresher Students of 2023-24 on 21st September, 2023.
- 23 Delivered a lecture on the title "*Innovations lead the mankind*" at Cluster College meeting of Virudhunagar District for the UG Physics Students at Devanga Arts College, Aruppukkotai on 18.08.2023.
- 22 Acted as Evaluator for State Level Camp (Level-II), Tamilnadu (Dakshin Region) of Vidyarthi Vigyan Manthan - India's Largest Science Talent Search for New India Using Digital Devices (VVM) 2022-23 held on 28th & 29th January, 2023 at Mepco Schlenk Engineering College, Sivakasi
- 21 Delivered a special lecture in the title of "*Inventions and History of Physics*" at Government Arts and Science College, Nagercoil - 4 during the Physics Association meeting held on 01.04.2022.
- 20 Delivered a special lecture in the title of "*Innovations lead the Mankind*" at Pioneer Kumaraswamy College, Nagercoil 629 003 during the Physics Association meeting held on 28.02.2022.
- 19 Delivered a lecture in the title of "*Science and inventions rule the universe*" - a live science talk webinar conducted by Er. Perumal Manimekalai College of Engineering, Hosur 635 117 on 4th February, 2022.
- 18 Delivered a short live radio speech (10 minutes) at Kumari FM (101 MHz @ Kanyakumari District) regarding "*Sir C.V. Raman and his inventions for societal impacts*" on 21st November, 2021, i.e., on his Death Anniversary.
- 17 Delivered a lecture through online mode in the title of "*Scientific Innovations Swivels the globe*", at Department of Physics, Avinashilingam University, Coimbatore on 11th November 2021.
- 16 Delivered a talk in the title of "*Engineering Studies and entrance tests*" to the School teachers of Tirunelveli District through Online mode organized by District Employment and Training Centre, Tirunelveli on 7th September, 2021

- 15 Delivered a lecture in the title of *"Innovations lead the mankind"* - a live science talk webinar conducted by Er. Perumal Manimekalai College of Engineering, Hosur 635 117 on 27th January, 2021.
- 14 Delivered two sessions as resource person in the title of *"Innovations lead the mankind"* at University VOC College of Engineering, Thootukudi 628 008 during the Induction programme on 16th November, 2020, FN through online mode.
- 13 Delivered a talk as resource person in the title of *"Science and Innovation"* at Anna University Regional Campus - Tirunelveli, Tirunelveli - 7 during the Induction programme on 16th November, 2020, AN through online mode.
- 12 Organised an international webinar on *"Scientific Advancements on Solutions and Testings in Industry"* through google meet live meeting and youtube live for 462 registered participants on August 10, 2020 as convener.
- 11 Deliver a talk in the title of *"Engineering Studies and entrance tests"* to the School students of Tirunelveli District through Online mode organized by District Employment and Training Centre, Tirunelveli on 13th July, 2020
- 10 Delivered a lecture in the title of *"Associate through Physics & Rule the Universe"*, at Department of Physics, Nesamony Memorial Christian College, Marthandam 629 165 on 16th March 2020
- 9 Delivered three sequential radio speeches at Kumari FM (101 MHz @ Kanyakumari District) regarding *"God's Particle"* during May 2018 (14.05.2018, 21.05.2018 & 28.05.2018)
- 8 Organised students activities, viz., Quiz, Competition, Elocution among the first year students in view of the celebration of world student's day - *a tribute to our people's president and "great soul" of India, Dr. A.P.J. Kalam* on 14.10.2017
- 7 Delivered a lecture in the title of *"Simply be a Physicist"*, at Department of Physics, Rajas' College, Rajapalayam 626 117 on 19th August 2017
- 6 Delivered a lecture in the title of *"Innovations leads the society"*, at Department of Physics, Sri Parasakthi College, Courtallam 627 802 on 28th February 2017
- 5 Coordinated Kanyakumari District Level Skill Summit-2017 with Tamil Nadu Skill Development Corporation on 04.10.2017
- 4 Coordinated the science exhibition for school children and for UCEN college students in the title of *"Exhibition of Science and Technology for Innovative Modern Applications - 2016 (ESTIMA 2016)"* on 27.02.2016.
- 3 Organized science lectures and expo competition for college year first students in the title of *"Udhayam"* in view of the science day celebrations on 23.03.2015
- 2 Organized a National level conference *"Advances in Materials (AIM 2014)"* on 07.10.2014
- 1 Coordinated a technological expo, namely TechUCEN to promote Kanyakumari Industries and students Innovations on 07.10.2013 & 08.10.2013

List of Publications in peer-reviewed journals

183. *Polymorphism in Chloride Salt of m-Nitroaniline: Structural, Spectroscopic, Thermal,*

- Molecular Docking, Biological, and Quantum Chemical Computational Investigation*, S. Thangarasu, V. Siva, S. Kannan, S. Asath Bahadur & **S. Athimoolam** (2023). *Polycyclic Aromatic Compounds*, 43(8), 7164-7181.
182. *Structural, vibrational and electro-optical properties on perchlorate salt of 4-methoxyaniline studied through experimental and theoretical methods*, V. Siva, A. Shameem, A. Murugan, S. Thangarasu, S. Asath Bahadur & **S. Athimoolam** (2023). *Polycyclic Aromatic Compounds*, 43(6), 4984-5000.
181. *Insight with Crystallization, Quantum Computation, Hirshfeld, ELF/ LOL and Molecular Docking of Syringic Acid Nicotinamide Cocrystal as Potent Mycobacterium Tuberculosis Inhibitor*, Azar Zochedh, **Athimoolam Shunmuganarayanan** & Asath Bahadur Sultan (2023). *J. Comput. Biophys. Chem.* 2023, 1-24
180. *Evaluation of drug likeliness of (Z)-4-((4-hydroxy-3-methoxy benzylidene)amino)-1,5-dimethyl-2-phenyl-1,2-dihydro-3H-pyrazol-3-one by computational analysis against coronavirus and T-cells of immune system*, Gowri M & Athimoolam S (2023). *Indian Journal of Chemistry*, 62, 559-567.
179. *Exploring the Synergistic Effect of Tegafur-Syringic Acid Adduct Against Breast Cancer through DFT Computation, Spectroscopy, Pharmacokinetics and Molecular Docking Simulation*, Azar Zochedh, Kaliraj Chandran, **Athimoolam Shunmuganarayanan** & Asath Bahadur Sultan (2023). *Poly. Arom. Compnds.*, 1-35.
178. *Combinatorial Effect of Syringic Acid-Pyrazinamide Adduct against Luminal Type Breast Cancer Investigated through DFT, Drug-Likeness, and Molecular Docking Simulation*, Mohana Priya, Azar Zochedh, Karthikeyan Palaniyandi, **Athimoolam Shunmuganarayanan** and Asath Bahadur Sultan (2023). *Poly. Arom. Compnds.*, 1-29.
177. *Experimental and computational studies of organic 4-[[4-chlorophenyl]imino]methyl]phenol single crystals for optic and biological applications*, C. Smitha Rose, T. Suthan, S. Mary Delphine, C. Cynitha Wise Bell & **S. Athimoolam** (2023). *J. Mol. Struct.* 1288, 135779.
176. *Antitumor and antimicrobial effect of syringic acid urea cocrystal: Structural and spectroscopic characterization, DFT calculation and biological evaluation*, Azar Zochedh, Mohana Priya, Athimoolam Shunmuganarayanan & Thandavarayan Kathiresan (2023). *J. Mol. Struct.* 1282, 135113.
175. *Conformational fidelity and hydrogen bond associability of L-histidine with sulfamate anion studied through XRD, quantum chemical, spectroscopic and molecular docking simulation as a cdk-4 inhibitor against retinoblastoma*, Azar Zochedh, **Athimoolam Shunmuganarayanan** & Asath Bahadur Sultan (2023). *J. Mol. Struct.* 1274, 134402.
174. *Structural, Spectroscopic, Cytotoxicity and Molecular Docking Studies of Charge Transfer Salt:4-Aminiumantipyrine Salicylate*, S. Thangarasu, A. Chitradevi, V. Siva, A. Shameem, A. Murugan, T. M.Viswanathan, **S. Athimoolam** & S. Asath Bahadur (2023). *Polycyclic Aromatic Compounds*, 43(4), 3159-3174.

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154. Participated and presented a paper, L. Mary Novena and **S. Athimoolam**, 2nd

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153. *"Nanocrystalline Quaternary $Cu_2ZnSnSe_4$ Thin Film for Sola Cell application"*, A. Murugan, V. Siva, A. Shameem, **S. Athimoolam** and S. Asath Bahadur, National Conference on Recent Developments in Effective Materials - REDEEMS'20, 7thFebruary 2020organized by Department of Physics, Sarah Tucker College, Tirunelveli, pg. 157. [ISBN 978-93-5396-426-9]
152. *"Thermal and antimicrobial studies on nitrate salt of 3-nitroaniline"*, S. Thangarasu, V. Siva, S. Asath Bahadur and **S. Athimoolam**, National Conference on Recent Developments in Effective Materials - REDEEMS'20, 7thFebruary 2020organized by Department of Physics, Sarah Tucker College, Tirunelveli, pg. 156. [ISBN 978-93-5396-426-9]
151. *"Orbital analysis of Hirshfield surface study of 4-methoxyanilinium perchlorate : a nonlinaer optical material"*, V. Siva, A. Shameem, A. Murugan, **S. Athimoolam** and S. Asath Bahadur, National Conference on Recent Developments in Effective Materials - REDEEMS'20, 7thFebruary 2020organized by Department of Physics, Sarah Tucker College, Tirunelveli, pg. 156. [ISBN 978-93-5396-426-9]
150. *"A computational study on structure and improved bioactivity of nitrate salt of vitamin B3 (Nicotinic acid)"*, M. Mary Latha, L. Mary Novena and **S. Athimoolam**, National Conference on Recent Developments in Effective Materials - REDEEMS'20, 7thFebruary 2020organized by Department of Physics, Sarah Tucker College, Tirunelveli, pg. 150. [ISBN 978-93-5396-426-9]
149. *"Solubility and biological studies of the co-crystal of Theophylline (a Bronchodialator drug) with resorcinol and pyrogallol"*, L. Mary Novena and **S. Athimoolam**, National Conference on Recent Developments in Effective Materials - REDEEMS'20, 7thFebruary 2020organized by Department of Physics, Sarah Tucker College, Tirunelveli, pg. 149. [ISBN 978-93-5396-426-9]
148. *"Hirshfel and Mulliken charge analysis of pharmaceutical cocrystals of Theophylline (a Bronchodilator drug)"*, L. Mary Novena and **S. Athimoolam**, National Conference on Recent Developments in Effective Materials - REDEEMS'20, 7thFebruary 2020organized by Department of Physics, Sarah Tucker College, Tirunelveli, pg. 148. [ISBN 978-93-5396-426-9]
147. *"Computational studies of an anticancer drug molecule: Midostaurin"*, **S. Athimoolam**, National Conference on Recent Developments in Effective Materials - REDEEMS'20, 7thFebruary 2020organized by Department of Physics, Sarah Tucker College, Tirunelveli, pg. 132. [ISBN 978-93-5396-426-9]
146. *"Theoretical and experimental vibrational spectroscopic investigation on nicotinamidium oxalate"*, E. Arockia Jeya Yasmi Prabha and **S. Athimoolam**, National Conference on Recent Developments in Effective Materials - REDEEMS'20, 7thFebruary 2020 organized by Department of Physics, Sarah Tucker College, Tirunelveli, pg. 24-27. [ISBN 978-93-5396-426-9]
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