



TO MAGNIFICO RETTORE OF UNIVERSITA' DEGLI STUDI DI MILANO

ID CODE Id-5953

## DR. SUBASHCHANDRABOSE SUBRAMANIYAN

I the undersigned asks to participate in the public selection, for qualifications and examinations, for the awarding of a type B fellowship at the Dipartimento di " PHYSICS "

Scientist- in - charge:

**Prof. Achilli Simona**

Project Title:

"Ab initio calculation of the properties of ZrTe<sub>3</sub> associated to the formation of a charge density wave, supporting experimental evidences"

### CURRICULUM VITAE

**Dr. SUBASHCHANDRABOSE SUBRAMANIYAN**

#### 1. PERSONAL INFORMATION

Surname	SUBRAMANIYAN
Name	SUBASHCHANDRABOSE

#### 2. PRESENT OCCUPATION

Appointment	Structure
TEMPRARORY Dec, 2019-Till date	RESEARCH- ASSOCIATE PROFESOR Head of the department of Physics, at the PRIST Deemed University, Thanjavur, TN, India

#### 3. EDUCATION AND TRAINING

Degree	Course of studies	specialization	University	year of achievement of the degree
1. M.SC	MASTER OF SCIENCE IN PHYSICS	PHYSICS	ANNAMALAI UNIVERSITY, TN, INDIA	2007
2. M.PHIL	MASTER OF PHILOSOPHY IN PHYSICS	ATOMIC AND MOLECULAR SPECTROSCOPY	ANNAMALAI UNIVERSITY, TN, INDIA	2009
3. PH.D	PHD IN PHYSICS	MOLECULAR STRUCTURE OF HETEROCYCLIC AND SCHIFF BASE COMPOUNDS- EXPERIMENTAL AND DFT APPROACH	ANNAMALAI UNIVERSITY, TN, INDIA	AUG,2012
Degree of medicalspecialization	-	-	-	-
Degree of Europeanspecialization	-	-	-	-



## 4. REGISTRATION IN PROFESSIONAL ASSOCIATIONS

Date of registration	Association	City
-	-	-

## 5. FOREIGN LANGUAGES

Languages	level of knowledge
TAMIL	Mother Tongue
ENGLISH	GOOD COMMUNICATION, READING AND WRITING
RUSSIAN	BASICS
ITALIAN	BASICS [LEARNING LEVEL]

## 6. AWARDS, ACKNOWLEDGEMENTS, SCHOLARSHIPS

Year	Description of award
2019-2021	Designation: Post-doc fellow Type (A) research grant Department of Physics and Astronomy "Galileo Galilei" University of Padova   Padova, Italy
2016-2018	Russian academic excellence 5 to 100 top projects. Science and Technology park «Fabrika», Immanuel Kant Baltic Federal University, (IKBFU), Gaydara st., 6, Kaliningrad, Russia
2023- Till date	Head of the department of Physics, Institution innovation council coordinator at the PRIST Deemed University, TN, India
22 <sup>nd</sup> MARCH 2014	Honoured as the best teacher and head of the department of science and Humanities - this award presented by Dr. K.Sivan, Director Indian space research organisation (ISRO), at the M.A.R. college of Engineering and Technology, on 22 <sup>nd</sup> March, 2014 at Trichy, Tamilnadu, India.
2012	I received best researcher award for having high publication during PhD at department of Physics, Annamalai University, TN India. (meritorious-scholarships)
2009	For blood donation (GOVT. HOSPITAL, CUDDALORE, TN, INDIA)

## 7. TRAINING OR RESEARCH ACTIVITY

description of activity: One week research training school and international conference participation	
WORKSHOP - 26- 30 <sup>th</sup> Nov-2018 Workshop-Indo-French School cum Conference on Magnetism of Molecular Systems   Indian Institute of Science, Bangalore - 560 012, India	
International conference: 20-24, August- 2017 International Baltic Conference on Magnetism focused of functionalized magnetic structure for energy and biomedical application. Kaliningrad, Russia	

## 8. PROJECT ACTIVITY

Year	Project
2023 Awaiting for results	ACCEPTED FOR EVALUATION STAGE-SERB/DST/GOVT. OF INDIA Design, development and investigation of 2D Dichalcogenide materials for photoelectric and tribological applications using the first principle approaches FILE NUMBER:EEQ/2023/000652



2019-2021	Type (A) research grant Developing computational codes, performing first principle calculations and Investigations Prof. Pier Luigi Silvestrelli Department of Physics and Astronomy “Galileo Galilei” University of Padova  Padova, Italy
2016-2018	Russian academic excellence 5 to 100 top projects Functionalized magnetic nano materials for energy and Biomedical applications Prof. Michael Farle, University of Duisburg-Essen  Chairman of the Magnetism, Germany. Science and Technology park «Fabrika», Immanuel Kant Baltic Federal University (IKBFU), Gaydara st., 6, Kaliningrad, Russia

## 9. PATENTS

Patent
WORKING ON IT

## 10. CONGRESSES AND SEMINARS: ORGANISED

Date	Title	Place
19-21 <sup>st</sup> , Feb, 2019	International conference on advance Chemicals and Structural Biology- Department of Science and Technology, SERB	PRIST Deemed University, Thanjavur, TN, India.
2 <sup>nd</sup> July 2016	Molecular simulation and interpretation of Chemical Structures (MSICS)- PRIST Deemed University & Indian Institute of Food Corporation of India	PRIST Deemed University, Thanjavur, TN, India.

## 11. CONGRESSES AND SEMINARS: INVITED TALK PRESENTED

Date	Title	Place
03 <sup>rd</sup> -04 <sup>th</sup> October 2023	Invited talk on: Screening and anti- screening effect in Fullerene cages	TBML Arts and Science College, Poraya, TN, India
23 <sup>rd</sup> -24 <sup>th</sup> August 2022	Invited talk on: Tunable van der Waals interactions in low-dimensional nanostructures, at ICMSSE, Holy cross college, Trichy, India.	Holy cross college, Trichy, TN, India.
28-30 <sup>th</sup> January 2016	Invited talk on: Interpretation of spectral, chromatographic, crystallographic and computational data of chemical system,	PRIST Deemed to be University, Thanjavur, TN, India



## 12. PUBLICATIONS:

**Total research publications (Dr. Subashchandraboze Subramaniyan):**

Total papers	Citations	h-index	i-index
50	643	15	21

## 1# Selective publications:

S.No	Title, Authors, Journals, Volume, Year an Pages
1.	Screening and anti-screening in fullerene-like cages: dipole-field amplification with ionic nanocages, Pier Luigi Silvestrelli, S Subashchandraboze, A Seif, Alberto Ambrosetti, Carbon Trends 10 (2023) 100242
2.	Tunable van der Waals interactions in low-dimensional nanostructures, Pier Luigi Silvestrelli S. Subaschandraboze, Alberto Ambrosetti, B. Liu, The Journal of Chemical Physics, 154 (2021) 224105
3.	Synthesis and characterization of poly indole-iron oxide nanoparticles for biomedical applications” Journal of Cluster Science article in press (2022)
4.	Electrochemical and magnetic properties of zinc ferrite nanoparticles through chemical co-precipitation method, K Sathiyamurthy, C Rajeevgandhi, S Bharanidharan, P Sugumar, S Subashchandraboze, Chemical Data Collections, 28 (2021) 100477.
5.	Synthesis, characterization and electrical conductivity of Fe <sub>3</sub> O <sub>4</sub> nanoparticles, B. Aarthy, S. Subashchandraboze*, J.S. Nirmal Ram, D. Nandhini, N. Anandhan, Indian Journal of Applied Research, (2019).
6.	Synthesis, characterization and computation of potassium doped calcium hydroxide nanoparticles and nanotubes, D Nandhini, S Subashchandraboze, P Ramesh, International Journal of Mechanical and Production Engineering Research and Development, Vol. 9, Issue 1, 441-448 (2019)
7.	Synthesis and Characterization of Ni Doped CuO Nanoparticles from Aqueous Solution, D Nandhini, S Subashchandraboze, International Journal of Current Engineering and Scientific Research, (2017)
8.	Single crystal, spectral and electronic transition studies on (E)-N-(3-methoxy-4- hydroxybenzylidene)-4-nitrobenzohydrazide monohydrate, M.Manvizhi, S.Murugan, S.Subaschandraboze P.Sutharsan, J.S.Nirmalram, Journal of Molecular structure, 1183 (2019) 390-397.
9.	Synthesis, crystal growth, structural evaluation and nonlinear optical analysis of ethyl-4- (3, 4-dimethoxyphenyl)-6-methyl-2-sulfanylidene-3, 4-dihydro-1H-pyrimidine-5- carboxylate, A Dhandapani, S Manivarman, S Subashchandraboze, Journal of Molecular Structure, 1127 (2017) 212-225.
10.	Crystal structure of ethyl (2S)-9-methoxy- 2-methyl-4-oxo-3,4,5,6-tetrahydro-2H- 2,6-methanobenzo[g][1,3,5]oxadiazocine- 11-carboxylate, Dhandapani, Manivarman, Subashchandraboze, Acta Cryst. E, 71 (2015) o117-o118
11.	FT-Raman, FT-IR spectra and total energy distribution of 3-pentyl-2, 6- diphenylpiperidin-4-one: DFT method, S Subashchandraboze, H Saleem, Y Erdogdu, G Rajarajan, V Thanikachalam, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 82 (2011) 260-269.
12.	Haemostatic effects of latex from Croton sparsiflorus Morang, in vitro, in vivo, in silico approaches, MC Kamaraj, S Mohan Raj, D Palani Selvam, S Subashchandraboze, A Kalaiselvan, Computational Biology and Chemistry, 74 (2018) 157-166.



13.	Investigation on the isoform selectivity of novel kinesin-like protein 1 (KIF11) inhibitor using chemical feature based pharmacophore, molecular docking, and quantum mechanical studies, Subramanian Karunakaran, Subramanian Subhashchandra Bose, Keun Woo Lee, Chandrasekaran Meganathan, Computational Biology and Chemistry, 61(2016) 47-61.
14.	Pharmacophore modeling, virtual screening, molecular docking studies and density functional theory approaches to identify novel keto hexokinase (KHK) inhibitors, Chandrasekaran Meganathan Rengarajan Kavitha, Subramanian Karunakaran, Subramanian Subhash Chandrabose, Keun Woo Lee, BioSystems 138 (2015) 39-52.
15.	Synthesis, in vitro and in silico antitumor evaluation of 3-(2, 6-dichlorophenyl)-1, 5-diphenylpentane-1, 5-dione: Structure, spectroscopic, RDG, Hirshfeld and DFT based analyses, A Dhandapani, S Veeramanikandan, Raju Suresh Kumar, Abdulrahman I Almansour, Natarajan Arumugam, S Subashchandra Bose, J Suresh, R Arulraj, D Gajalakshmi, Journal of Molecular Structure, 1251 (2022) 132002.
16.	Spectroscopic, structural, electronic and bioactive characteristics of 3, 5-bis (2, 5-dimethylphenyl) pyridine (1): An experimental and theoretical investigations, Muhammad Akram, Shanawer Niaz, Muhammad Adeel, Muhammad Nawaz Tahir, Irfan Ullah, Malik Aman Ullah, S Subashchandra Bose, Ghias Uddin, Journal of Molecular Structure, 1203 (2020) 127448
17.	Synthesis, solid state structure, Hirshfeld surface, nonlinear optics and DFT studies on novel bischalcone derivative, Synthesis Veeramanikandan, H Benita Sherine, A Dhandapani, S Subashchandra Bose, Journal of Molecular Structure, 1180 (2019) 798-811
18.	Synthesis, rotational, vibrational and transitional spectra investigation on novel ethyl-4-(3-(benzo [d] 1, 3di-oxole-5-carboxamido) phenyl)-1, 2, 3, 4-tetrahydro-6-methyl-2, C Adaikalaraj, S Manivarman, S Subashchandra Bose, A Dhandapani, Journal of Molecular Structure, 1165 (2018) 132-141.
19.	Synthesis, Spectroscopic, Intramolecular Energy Transfer and Electronic Structure Nonlinear Optical Properties of Novel Tetrahydropyrimidinone, Ukkaramoorthy Umadevi, Arumugam Dhandapani, Subramanian Manivarman, Subramanian Subashchandra Bose, Oriental Journal of Chemistry, 34 (2018) 1222
20.	Synthesis and spectral characterization of bis (4-amino-5-mercapto-1, 2, 4-triazol-3-yl) propane, S Subashchandra Bose, V Thanikachalam, G Manikandan, H Saleem, Y Erdogdu, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 157 (2016) 96-103.
21.	Structural and vibrational studies on 1-(5-methyl-[1, 3, 4] thiadiazol-2-yl)-pyrrolidin-2-ol, N Ramesh Babu, H Saleem, S Subashchandra Bose, M Syed Ali Padusha, S Bharanidharan, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 152 (2016) 252-261.
22.	Vibrational studies on (E)-1-((pyridine-2-yl) methylene) semicarbazide using experimental and theoretical method, S Subashchandra Bose, N Ramesh Babu, H Saleem, M Syed Ali Padusha, Journal of Molecular Structure, 1094 (2015) 254-263.
23.	Synthesis and spectroscopical study of rhodanine derivative using DFT approaches, R Anbarasan, A Dhandapani, S Manivarman, S Subashchandra Bose, H Saleem, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 146 (2015) 261-272.
24.	Vibrational spectroscopy investigation and density functional theory calculations on (E)-N'-(4-methoxybenzylidene) benzohydrazide, H Saleem, S Subashchandra Bose, N Ramesh Babu, M Syed Ali Padusha, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 43 (2015) 230-241.



25.	Synthesis and spectral characterization of hydrazone derivative of furfural using experimental and DFT methods, N Ramesh Babu, S Subashchandrabose, M Syed Ali Padusha, H Saleem, YUSUF Erdogan, <i>Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy</i> , 120 (2014) 314-322.
26.	Molecular structure and vibrational analysis on (E)-1-(3-methyl-2, 6-diphenyl piperidin-4-ylidene) semicarbazide, A Dhandapani, S Manivarman, S Subashchandrabose, H Saleem, <i>Journal of Molecular Structure</i> , 1058 (2014) 41-50.
27.	Vibrational and conformational analysis on-N1-N2-bis ((pyridine-4-yl) methylene) benzene-1, 2-diamine, S Subashchandrabose, C Meganathan, YUSUF Erdogan, H Saleem, C Jajkumar, P Latha, <i>Journal of Molecular Structure</i> , 1034 (2013) 37-44.
28.	FT-IR, FT-Raman spectral and conformational studies on (E)-2-(2-hydroxybenzylidenamino)-3-(1H-indol-3yl) propionic acid, H Saleem, S Subashchandrabose, Y Erdogan, V Thanikachalam, J Jayabharathi, <i>Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy</i> , 101 (2013) 91-99.
29.	Structural and vibrational studies on (E)-2-(2-hydroxy benzyliden amino)-3-phenyl propionic acid using experimental and DFT methods, H Saleem, Y Erdogan, S Subashchandrabose, V Thanikachalam, J Jayabharathi, N Ramesh Babu, <i>Journal of Molecular Structure</i> , 1030 (2012) 157-167.
30.	FT-Raman, FT-IR spectral and DFT studies on (E)-1-4-nitrobenzylidenethiocarbonohydrazide, V Thanikachalam, V Periyannayagasamy, J Jayabharathi, G Manikandan, H Saleem, S Subashchandrabose, Y Erdogan, <i>Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy</i> , 87 (2012) 86-95.
31.	Structural, vibrational and hyperpolarizability calculation of (E)-2-(2-hydroxybenzylideneamino)-3-methylbutanoic acid, Subashchandrabose, H Saleem, Y Erdogan, Ö Dereli, V Thanikachalam, J Jayabharathi, <i>Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy</i> , 86 (2012) 231-241.
32.	Density functional theory studies on 2, 5-bis (4-hydroxy-3-methoxybenzylidene) cyclopentanone, H Saleem, Akhil R Krishnan, Y Erdogan, S Subashchandrabose, V Thanikachalam, G Manikandan, <i>Journal of Molecular Structure</i> , 999(2011)2-9.
33.	FT-IR, FT-Raman spectra and scaled quantum mechanical study of 4-amino-1-benzylpiperidine, S Chandra, H Saleem, Y Erdogan, S Subashchandrabose, Akhil R Krishnan, MT Gulluoglu, <i>Journal of Molecular Structure</i> , 998(2011)69-78.
34.	Synthesis and comparison of bis (4-amino-5-mercapto-1, 2, 4-triazol-3-yl) butane using DFT study, S Subashchandrabose, Akhil R Krishnan, H Saleem, S Kavitha, V Thanikachalam, G Manikandan, <i>Journal of Molecular Structure</i> , 996(2011)1-11.
35.	Molecular structure, vibrational spectroscopic (FT-IR, FT-Raman), UV and NBO analysis of 2-chlorobenzonitrile by density functional method, Akhil R Krishnan, H Saleem, S Subashchandrabose, N Sundaraganesan, S Sebastain, <i>Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy</i> , 78(2011)582-589.
36.	Vibrational spectroscopic study and NBO analysis on bis (4-amino-5-mercapto-1, 2, 4-triazol-3-yl) methane using DFT method, <i>Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy</i> , S Subashchandrabose, Akhil R Krishnan, H Saleem, R Parameswari, N Sundaraganesan, V Thanikachalam, G Manikandan, 77 (2010) 877-884.
37.	FT-IR, FT-Raman, NMR spectral analysis and theoretical NBO, HOMO-LUMO analysis of bis (4-amino-5-mercapto-1, 2, 4-triazol-3-yl) ethane by ab initio HF and DFT methods, S Subashchandrabose, Akhil R Krishnan, H Saleem, V Thanikachalam, G Manikandan, Yusuf Erdogan, <i>Journal of Molecular Structure</i> , 981(2010)59-70.

\*corresponding author



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<https://www.scopus.com/authid/detail.uri?authorId=36247723600>

<b>2# Articles in reviews</b>
Title: Synthesis and characterization of poly-indole iron oxide nanoparticles for biomedical applications
Journal: Inorganic Chemistry communication
Status: Under revision

### 13. OTHER INFORMATION

1	<b>Professional skill</b>	
	<b>1#Teaching Experience</b>	
	1# Position	Scientist and Head, Associate Professor of Physics
	Service period	18-12-2021-Till date  24months
	Role	Research/Teaching
	Institute	Research and Development Cell (RDC)   PRIST Deemed University, Thanjavur, Tamilnadu-613403
	Country	India
	2# Position	Associate Professor
	Service period	July, 2018-December, 2019  18 months
	Role	Guiding PhD, Master students, Teaching to the Master students and Research work
	Institute	Centre for Research and Development (CRD)   PRIST Deemed University, Thanjavur, Tamilnadu-613403
	Country	India
	3#Position	Assistant Professor and Scientist
	Service period	3rd September, 2014- 30th December, 2016  26 months
	Role	Research work, Teaching to the Master, Guiding PhD, and Master
	Institute	Centre for Research and Development (CRD)   PRIST Deemed University, Thanjavur, Tamilnadu-613403
	Country	India
	4# Position	Assistant Professor and Head
	Service period	March, 2012- 30th June, 2014  ( 27 months)
	Role	Research work & Teaching to the Bachelor of Engineers (B.E)
	Department	Department of Science and humanities
	Institute	M.A.R. College of Engineering and Technology   Trichy   Tamilnadu   621316
	Country	India-621316
2#Programming	<ul style="list-style-type: none"> <li>➤ FORTRAN 95</li> <li>➤ Python (Learning)</li> </ul>	
3#Experience in comp. codes	➤ Quantum Espresso  Wein2K_17.1  Gaussian 03, 09  VESTA	
4#Computational resources	➤ CINECA-ISCRA (Italian Super Computing Resource Allocation)	



	4#Description of Scientific experience	<ul style="list-style-type: none"> <li>➤ State-of-the-art first-principle simulation techniques</li> <li>➤ First-principle calculations on 1D and 2D nano structures</li> <li>➤ Computational code development</li> <li>➤ Organic single crystals-growth and structure solutions</li> <li>➤ Synthesis of nanomaterials (especially using sol-gel method) and preparation of precursors.</li> <li>➤ Scientific instruments handled- FT-IR, FT-Raman, UV-Visible, X-ray, and FE-SEM and SEM-EDX</li> </ul>														
	3#Software developed	<ul style="list-style-type: none"> <li>➤ MBD code &amp; Interface code developed for generating input files, to calculate the binding energy and power law</li> <li>➤ Link to a repository: <a href="https://github.com/sscbphysics/qhorec">https://github.com/sscbphysics/qhorec</a></li> </ul>														
<b>Research supervision and leadership experience</b>																
2	1#As a Supervisor	I was being as supervisor for Ph.D scholar; There are two scholars have completed PhD under my supervision														
	Thesis Title 1	Growth and characterization of organic and semi-organic functional non-linear single crystals														
	Thesis Title 2	Synthesis and characterization of Cu and Ni doped iron oxide and alkali metals doped Ca(OH) <sub>2</sub> nanoparticles for energy and biomedical applications														
	2#As a Head	I was serving as a Head for Department of Science and Humanities at the M.A.R college of Engineering and Technology, TN, India.														
<b>Other key academic merits</b>																
3	1#Referee of Scientific journals	<table border="0"> <tr> <td>J.Mol.Struct.</td> <td>  Journal of Molecular Structure</td> </tr> <tr> <td>Arb.J.Chem.</td> <td>  Arabian journal of chemistry</td> </tr> <tr> <td>Solid-state elect.</td> <td>  Solid-state electronics</td> </tr> <tr> <td>Comp.Mat.Sci.</td> <td>  Computational Materials Science</td> </tr> <tr> <td>Chem.phys.Lett</td> <td>  Chemical Physics Letters</td> </tr> <tr> <td>Spectrochim Acta A</td> <td>  Molecular and Bimolecular Spectroscopy</td> </tr> <tr> <td>J.Mol.Struct.</td> <td>  Journal of Molecular liquids</td> </tr> </table>	J.Mol.Struct.	Journal of Molecular Structure	Arb.J.Chem.	Arabian journal of chemistry	Solid-state elect.	Solid-state electronics	Comp.Mat.Sci.	Computational Materials Science	Chem.phys.Lett	Chemical Physics Letters	Spectrochim Acta A	Molecular and Bimolecular Spectroscopy	J.Mol.Struct.	Journal of Molecular liquids
		J.Mol.Struct.	Journal of Molecular Structure													
Arb.J.Chem.	Arabian journal of chemistry															
Solid-state elect.	Solid-state electronics															
Comp.Mat.Sci.	Computational Materials Science															
Chem.phys.Lett	Chemical Physics Letters															
Spectrochim Acta A	Molecular and Bimolecular Spectroscopy															
J.Mol.Struct.	Journal of Molecular liquids															
4	Other education and expertise	One year “Computer - Cum- Internet Literacy Programme” by the Directorate of Collegiate Education, Department of Higher Education, Government of India. 2001-2002														
5	Personal information	Date of Birth: 27.05.1983														
		Place of Birth: Chidambaram														
		Address: Sagajanantha nagar, Parathur & Post, Chidambaram Taluk, Cuddalore District Tamilnadu (TN)-608201, India														

Declarations given in the present curriculum must be considered released according to art. 46 and 47 of DPR n. 445/2000.

The present curriculum does not contain confidential and legal information according to art. 4, paragraph 1, points d) and e) of D.Lgs. 30.06.2003 n. 196.

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Place and date: Thanjavur, Tamilnadu, India, 08-11-2023,