FACULTY PROFILE

Name: Dr. K. senthilkumar

Designation: Associate Professor

Contact Details: Department of Physics, Bharathiar University, Coimbatore- 641 046

Address: 47, Muthusaral Nagar, Kalveerampalayam, Bharathiar University (PO), Coimbatore – 641 046

Employee Number: 593

Date of Birth: 06. 05. 1975

Contact Phone (Office) : +91 (0)422 - 2428448 **Contact Phone** (Mobile) : +91 9486411335

Contact e-mail(s) : ksenthil@buc.edu.in

1 Education

S.No	Degree	Subject	Institution	Affiliated University	Year of Passing	Class/Grade
1	Ph.D.	Physics	Bharathiar University	Bharathiar University	2002	Highly commended
2	M.Phil.	Physics	Bharathiar University	Bharathiar University	1999	Commended
3	M.Sc.	Physics	Bharathiar University	Bharathiar University	1997	First Class
4	B.Sc.	Physics	Bharathiar University	Bharathiar University	1995	First Class

1.1 NET/SET/GATE/Others

S.No	Name of the Examination	Year of Passing	Register Number

2 Career Profile

S.No.	Institution	Designation	Period		Total Period in Years
			From	To	
1	Bharathiar University	Associate Professor	2018	Till date	2 Years & 2 Months
2	Bharathiar University	Associate Professor	2008	2017	10 Years
3	N.G.M. College, Pollachie	Lecturer in Physics	2006	2008	1 Year & 4 Months
4	Bristol University< UK	Post Doctoral Research Associate	2005	2006	1 Year & 4 Months
5	Delft University of Technology, The Netherlands	Post Doctoral Researcher	2002	2005	2 Years & 10 Months

3 Administrative / Additional Responsibilities

S.No.	Name of the Responsibility	Designation	Institution	Period		Nature of Responsibility
				From	To	
1	Data Center Coordinator	Data Center Coordinator	Bharathiar University	07.09.2011	Till date	Taking care of LAN and internet facility of entire University

5 Membership in Professional Bodies

Sl No.	Organization	Type of Membership	Period
1	Member – American Chemical Society	Regular Member	2015-2018

5.1 Membership in Academic Bodies

Sl No.	Organization	Type of Membership	Period

6. Visits/Exposure

Sl No.	Countries Visits	Duration of Visit	Month and Year	Purpose of Visit
1	China	7 days	June 2017	Visiting Scientist
2	Finland	6 days	June 2009	International Congress on Quantum Chemistry
3	UK	1 year	August 2005	Post Doctoral Research Associate
4	Germany	1 day	March 2005	Group Symposium on Molecular simulation
5	USA	6 days	June 2004	Sixth international symposium on functional Pi- electron systems
6	Sweden	15 days	August 2003	European Summer School in Quantum Chemistry
7	The Netherlands	2 years 10 months	August 2002	Post Doctoral Researcher
8	Italy	18 days	May 2001	Spring college in Numerical methods in electronic structure theory

7 Research Areas

Molecular Quantum Mechanics	✓ Electronic structure, molecular mechanics and dynamics calculations to study the structure, interactions and reaction mechanism ✓ Theoretical studies on charge transport and opto-electronic properties of π-stacked and conjugated organic systems ✓ Computational material science - applications include biocompatibility, catalytic activity, corrosion inhibition, opto-electronic and solar cell ✓ Quantum mechanical and molecular mechanical (QM/MM) studies on atmospheric and bio-chemical reactions

8 Supervising Profile

Year	M.Sc. (Nos)	M.Phil. (Nos)	Ph.D. (Nos)	PDF (Nos)	Others
2009	3	2	-	-	-
2010	2	3	2	-	-
2011	2	2	3	-	-
2012	2	3	4	-	-

2013	2	1	8	-	-
2014	2	1	6	-	-
2015	2	1	5	-	-
2016	2	1	6	-	-
2017	2	1	5	-	-
2018	3	1	4	-	-
2019	3	-	4	-	-
2020	2	-	5	-	-

8.1 PG research

S.No	Name of the Canditate	Title of the Dissertation	Year
25	I. Ajin	Effect of structural fluctuation on charge transport in π-stacked triphenylene derivatives - a theoretical study	2019
24	S.P. Keerthana	A density functional theory investigation on the reaction mechanism and thermochemistry of isoprene epoxydiols formation in the atmosphere	2019
23	K. Nandhakumar	Theoretical study on stacking angle fluctuations in TriB (Triphenyl Benzene) derivative using molecular dynamics simulation	2019
22	S. Ram Prakash	Effect of Stacking angle fluctuation on charge carrier mobility in pi- stacked Tris (N- Phenyltriazole)- A DFT Study	2019
21	U. Abdul Kareem	Molecular mechanics and molecular dynamics study on stacking distance and stacking angle in tris(n-Phenyltriazole) derivative	2018
20	T. Kiruthika	Theoretical study on Gas phase reaction of methyl chavicol with NO_3 radical	2018
19	K. Subramanyan	Computational insight into impact of stacking angle on charge transport in π	2017
18	T.P. Praseeda	Theoretical studies on the degradation mechanism of diuron through the reaction with OH radical	2017
17	J. Evangelin Princy	Structure, Interaction and adsorption spectra of fused imidazolium cation with BF_4^-, $CF_3SO_3^-$ anions	2016
16	G. Manonmani	Theoretical studies on the reaction of criegee intermediates CH_2OO and CH_3CHOO with water dimer	2016
15	N. Priya	Theoretical studies on interaction between stacked guanine-cytosine base pairs	2015

14	S. Bagyalakshmi	Adsorption ofTetracyanoquinodimethane and Tetrathiafulvalene on Al (100) surface: A First Principle Study	2015
13	S. Malarvizhi	Structural and Energetical Properties of 1-acyl-3-substituted Thiourea Isomers	2014
12	M. Rajeswari	A theoretical Study on the Structure and Stabilityof 3,5-bis-[2-3,4,5)-trimethyl-phenyl-vinyl]-1H-Pyrazole and its dimer	2014
11	R. Sahana banu	Mechnism and Kinetics of the Nitration of Tyrosine by O_3 and NO_2	2013
10	J. Shoba	Adsorption of Perfluropentacene on Al (100) Surface – A theoretical Study	2013
9	N. Vanitha Lakshmi	A Theoretical investigation on Adsorption of Pentacene on SiO_2 (100) Surface	2012
8	K. Mahalaksmi	Reaction Mechnism and Kinetics of the Oxidation of NO_2 by O_3 in the Atmosphere – Theoretical Study	2012
7	B. Sathyamoorthy	Theoretical studies on the atmospheric reactions of 2,3- dimethylphenol with OH radical	2011
6	C. Kalaiarasi	A theoretical study on structural and energetical properties of $(CrO_3)_n$ (n=1-5) and $(TiO_2)_n$ (n=1-4) clusters	2011
5	M. Vennila	Study of stacking angle in discotic liquid crystalline molecules THDP and THDDP using molecular dynamic simulations.	2010
4	S. Yuvarani	Potential energy surface characterization of HCCO+NO_2 reaction	2010
3	L. Sandhiya	Theoretical studies on dimers of barbituric acid.	2009
2	M. Kousalya	Density functional studies on structure, stability and optical absorption of unsubstituted and substituted 4-bromo-1-naphthyl chalcones.	2009
1	G. Vasugi	Effect of substitution and conformation on the stability of 4-bromo-1-naphthyl chalcones.	2009

8.2 M.Phil. Research

S.NO	Name of the Candidate	Title of Thesis	Year
17	K. Kanimozhi	Effect of stacking angle fluctuation on charge carrier mobility in π- stacked triazole based star shaped molecules	2018
16	S. Indhu	Theoretical study on the reaction mechanism and kinetics of sulfonylamine with water molecules	2017
15	M. Rajeswari	Opto-electronic and adsorption properties of azobenzene dyes on TiO_2 surface	2016
14	R. Jayabharathi	Theoretical Studies on the Mechanism and Kinetics of the Reaction of Terbacil with OH Radical	2015
13	N. Saranya	Theoretical studies on charge transport properties of 3,5 bis-[2-(3,4,5-trimethoxy –phenyl)-vinyl]-1H-pyrazole	2014
12	M.Gnanaprakasam	Mechanism and Kinetics of the Atmospheric oxidation of Naphthalene initiated by OH radical	2013
11	M. Sowmiya	Structural, optical and charge transport properties of cyclopentadithiophene derivatives: A theoretical study	2012
10	S. Ponnusamy	Studies on the mechanism, kinetics and global warming potential of the atmospheric degradation of perfluoropolymethylisopropyl ether by OH radical	2012
9	R. Deepika	Adsorption of pentacene on Pd(100) surface: structural and electronic properties from first principle study	2012
8	C. Kalaiarasi	Theoretical studies on charge transport properties on Ph4DP and Ph4DTP molecules	2012
7	S. Yuvarani	A theoretical study of structural and electronic properties of pentacene/Al(100) interface	2011

6	M. Vennila	Theoretical studies on the reaction mechanism of sulfadoxine with pi-acceptors	2011
5	G. Vasugi	Absorption and Emission properties of Borondipyrromethene dye and its substituted analogs	2010
4	A.Shanmugavani	Quantum chemical studies on structure and conformational stability of D-Sorbitol and D-Sorbitol-8H_2O complexes	2010
3	N. Lakshmi	Atmospheric reaction pathways and kinetics of the reaction of 1,4-thioxane with OH radical	2010
2	G. Saranya	Studies on charge transport in π -stacked liquid crystalline molecules THDP and THDDP.	2009
1	R. Nithya	Structural and spectral properties of 4-bromo-1-naphthyl chalcones-A quantum chemical study.	2009

8

3 Ph.D. research

Sl No	Name of the candidate	Supervisor/Co-Supervisor	Title of the Thesis	Number of Peer Reviewed Publications		Year
				National	International	
1	R. Bhuvaneswari	Dr. K. Senthilkumar	Computational perspective on the atmospheric oxidation of few volatile organic compounds initiated by hydroxyl radical		4	2020
2	M. Gnanaprakasam	Dr. K. Senthilkumar	Theoretical investigation on mechanism and kinetics of the atmospheric chemical reactions of few volatile organic compounds		5	2018
3	M. Sowmiya	Dr. K. Senthilkumar	Theoretical studies on interaction of molecules with anatase TiO2 (001) surface for medical, catalytic and dye sensitized solar cell applications		8	2017
4	S. Ponnusamy	Dr. K. Senthilkumar	Theoretical studies on the reaction mechanism and kinetics of atmospheric pollutants with hydroxyl radical		7	2017
5	K. Navamani	Dr. K. Senthilkumar	Charge Carrier Dynamics in Few π-stacked Organic Molecules		7	2015
6	L. Sandhiya	Dr. K. Senthilkumar	Theoretical studies on the mechanism and kinetics of atmospheric chemical reactions	1	8	2015
7	R. Nithya	Dr. K. Senthilkumar	Quantum chemical studies on the opto-electronic properties π-conjugated organic molecules		6	2014
8	G. Saranya	Dr. K. Senthilkumar	Quantum chemical studies on optical and charge transport properties of organic molecules and organic/metal Interfaces		9	2014

8.4 Postdoctoral research (RA/WOS/NPDF/Others

Sl No.	Name of the candidate	Title of the Thesis	Number of Peer Reviewed Publications		Year
			National	International	

9 Funded

S.No	Funding agency	PI	Title	Duration		Amount sanctioned	Amount received	Papers published if any	Ph.D. produced
				From	To				
1	DRDO	Dr. K. Senthilkumar	Theoretical studies on charge transport properties in organic field effect transistor	2009-2012		7.401 lakh	7.401 lakh	5	1
2	DST	Dr. K. Senthilkumar	Effect of structural fluctuations and environment on charge transport in π-stacked and conjugated organic molecules	2010-2012		17.872 lakh	17.872 lakh	5	1
3	UGC	Dr. K. Senthilkumar	Quantum mechanical and molecular mechanical studies on the reactions of pollutants in atmosphere and in water	2012 - 2015		13.438 lakh	13.438 lakh	5	1

10

S.No	Description	Duration	Amount Earned

11

S.No	Funding agency	Amount sanctioned	Amount received
		To	

12 Patents

S.No	International/National	Year	Application / Grant Number

13

S.No.	Funding agency	Duration	Title of the Project	Equipment purchased (Above 1 lakh)	Cost (Rs.in Lakhs)	Present Status
1	DST	3 years	Effect of structural fluctuations and environment on charge transport in π-stacked and conjugated organic molecules	High performance computing (HPC) facility	8.72	Working
2	NPO:L, DRDO	3 years	Theoretical studies on charge transport properties in organic field effect transistor	Four numbers of computing nodes for HPC	4	Working
3	UGC	3 years	Quantum mechanical and molecular mechanical studies on the reactions of pollutants in atmosphere and in water	Four numbers of computing nodes for HPC	7	Working

14 Publications

14.1 Resesarch articles in Journals (International)

S.No	Name of the authors	Title	Journal name	Volume	Pages	Year	SCI Indexed	Current Impact Factor	SJR	SNIP
103	G. Manonmani, L. Sandhiya and K. Senthilkumar	Hydrolysis of HNSO2: A Potential Route for Atmospheric Production of H2SO4 and NH3	Int. J. Quantum Chem	-	e26182	2020	Yes	2.263		
102	G. Manonmani, L. Sandhiya and K. Senthilkumar	Mechanism and kinetics of Diuron Oxidation by Hydroxyl Radical Addition Reaction	Environmental Science and Pollution Research	-	1	2020	Yes	2.914		

101	R. Bhuvaneswari and K. Senthilkumar	First Principle Studies on the Atmospheric Oxidation of HFC-C1436 Initiated by OH radical	New J. Chem	44	2070	2020	Yes	3.069		
100	R. Bhuvaneswari and K. Senthilkumar	A comprehensive quantum chemical study on the mechanism and kinetics of atmospheric reactions of 3-Chloro-2-methyl-1-propene with OH radical	Theor. Chem. Acc	139	Article no.2	2020	Yes	2.233		
99	K. Navamani, Swapan Pati, and K. Senthilkumar	Effect of Site Energy Fluctuation on Charge Transport in Disordered Organic Molecules	J. Chem. Phys	151	224301	2019	Yes	2.997		
98	G. Manonmani, L. Sandhiya and K. Senthilkumar	Mechanism and Kinetics of Diuron Oxidation Initiated by Hydroxyl Radical – Hydrogen and Chlorine Atom Abstraction Reactions	J. Phys. Chem. A	123	8954	2019	Yes	2.836		
97	M. Gnanaprakasam, G. Saranya, S. Bandaru, N. J. English and K. Senthilkumar	Atmospheric Oxidation Mechanism and Kinetics of 2-Bromo-4, 6-dinitroaniline by OH radical – A Theoretical Study	Phys. Chem. Chem. Phys	21	21109	2019	Yes	3.567		
96	P.V. Ravi, D. T. Thangadurai, D. Nataraj, K. Senthilkumar, G. Manonmani, N. Kalarikkal, S.	Graphene Nanobuds: A New Second-Generation Phosgene Sensor with Ultralow Detection Limit in Aqueous Solution	ACS Applied Materials & Interfaces	11	19339	2019	Yes	8.456		

	Thomas, P. Govindh									
95	R. Bhuvaneswari and K. Senthilkumar	Theoretical Study on the Gas Phase Reaction of Methyl Chavicol with Hydroxyl Radical	Computational and Theoretical Chemistry	78	1151	2019	Yes	1.403		
94	M. Gnanaprakasam, L. Sandhiya and K. Senthilkumar	Mechanism and Kinetics of the Oxidation of Dimethyl Carbonate by Hydroxyl Radical in the Atmosphere	Environmental Science and Pollution Research	26	3357	2019	Yes	2.914		
93	M. Vinodha and K. Senthilkumar	Adsorption of Tetracyanoquinodimethane and Tetrathiafulvalene on Aluminium (100) surface - A First Principle Study of Structural and Electronic Properties	Journal of Molecular Simulation	45	492	2019	Yes	1.782		
92	M. Gnanaprakasam, L. Sandhiya and K. Senthilkumar	Theoretical Investigation on the Mechanism and Kinetics of Atmospheric Reaction of Methyldichloroacetate with Hydroxyl Radical	J. Phys. Chem. A	122	9316	2018	Yes	2.836		
91	S. Ponnusamy, L Sandhiya and K. Senthilkumar	Atmospheric Oxidation Mechanism and Kinetics of Hydrofluoroethers CH3OCF3, CH3OCHF2 and CHF2OCH2CF3, by OH Radical: A Theoretical Study	J. Phys. Chem. A	122	4972	2018	Yes	2.836		
90	S. Krishnan and K. Senthilkumar	Theoretical probe on modified organic dyes for high-performance Dye-Sensitized Solar Cell	Current Applied Physics	18	1071	2018	Yes	2.010		

89	M. Gnanaprakasam, L. Sandhiya and K. Senthilkumar	Mechanism and kinetics of the reaction of methyl acetate with Cl atom – A theoretical study	Computational and Theoretical Chemistry	1131	40	2018	Yes	1.403		
88	S. Ponnusamy, L Sandhiya and K. Senthilkumar	Mechanism and Kinetics of the Degradation of Terbacil initiated by OH radical - A Theoretical Study	Chem. Phys	501	110	2018	Yes	1.822		
87	M. Vinodha and K. Senthilkumar	Counter anion effect on structural, opto-electronic and charge transport properties of fused π-conjugated imidazolium compound	Molec. Phys	116	1145	2018	Yes	1.704		
86	L Sandhiya and K. Senthilkumar	Exploring the Mechanisms for the Radical Induced Damage of 6-Thioguanine	Int. J. Quantum Chem	118	e25544	2018	Yes	2.263		
85	M. Gnanaprakasam, L. Sandhiya, K. Senthilkumar	A theoretical investigation on the mechanism and kinetics of the gas-phase reaction of naphthalene with OH radical	Theor Chem Acc	136	Article no. 131	2017	Yes	2.233		
84	K. E. Ranaghan, W. G. Morris, L. Masgrau, K. Senthilkumar, L. O. Johannissen, N. S. Scrutton, J. N. Harvey, F.	Ab initio QM/MM modelling of the rate-limiting proton transfer step in the deamination of tryptamine by aromatic amine dehydrogenase	J. Phys. Chem. B	121	9785	2017	Yes	2.923		

	R. Manby and A. J. Mulholland									
83	G. Bharathi, D. Nataraj, P. Sellan, M. Sowmiya, K. Senthilkumar, T. Daniel Thangadurai, O. Khyzhun, M. Gupta, D. Phase, N. Patra, S. Jha, and D. Bhattacharyya	Graphene quantum dot solid sheets: strong blue-light-emitting & photocurrent-producing band-gap-opened nanostructures	Nature - Scientific Reports 7	7	Article No. 10850,	2017	Yes	4.122		
82	S. Ponnusamy, L Sandhiya and K. Senthilkumar	Atmospheric oxidation mechanism and kinetics of 1, 3, 5-Trimethylbenzene initiated by OH radical - A theoretical study	New J. Chem	41	10259	2017	Yes	3.069		
81	T. Shanmugavadivu, K. Senthilkumar, P. Muthuraja, S. Balachandar and M. Sethu Raman	Theoretical and experimental evaluation of a new organic proton transfer crystal aminoguanidinium p-nitrobenzoate monohydrate for optical limiting applications	J. Phys. and Chem. of Solids	111	82	2017	Yes	2.048		
80	R. Bhuvaneswari, L. Sandhiya and K. Senthilkumar	Theoretical investigations on the mechanism and kinetics of OH radical initiated reactions of monochloroacetic acid	J. Phys. Chem. A	121	6028	2017	Yes	2.836		
79	M..Sowmiya and K. Senthilkumar	Opto-electronic and interfacial charge transfer properties of azobenzene dyes on Anatase	J. Photochemistry and Photobiology A: Chem	346	372	2017	Yes	3.261		

		TiO2 (001) surface -The effect of anchoring group								
78	M..Sowmiya and K. Senthilkumar	Conversion of toluene into benzyl radical on Anatase TiO2 (001) surface	Computational and Theoretical Chemistry	1115	13	2017	Yes	1.403		
77	S. Ponnusamy, L Sandhiya and K. Senthilkumar	Mechanism and kinetics of the reaction of nitrosamines with OH radical - A theoretical study	Int. J. Chem. Kin	49	339	2017	Yes	1.417		
76	R. Prabhakaran, P. Kalaivani, K. Senthilkumar and K. Natarajan	Synthesis, structural characterisation, DNA/ protein binding and in vitro cytotoxicity of three structurally different organoruthenium metallates from single pot	J. Organometallic Chem	83	825	2016	Yes	2.173		
75	M.Sowmiya and K. Senthilkumar	Dissociation of N2O on Anatase TiO2 (001) surface - The effect of oxygen vacancy and presence of Ag cluster	Applied Surface Science	389	1220	2016	Yes	5.155		
74	L Sandhiya, S. Ponnusamy and K. Senthilkumar	Atmospheric oxidation mechanism of OH-initiated reactions of diethyl ether – The fate of 1-ethoxy ethoxy radical	RSC Advances	6	81354	2016	Yes	3.049		
73	N. Selvakumaran, L. Sandhiya, N.S.P. Bhuvanesh, K. Senthilkumar and R. Karvembu	Structural diversity in aroylthiourea copper complexes – formation and biological evaluation of [Cu(I)(μ-S)SCl]2, cis-Cu(II)S2O2,	New J. Chem	40	5401	2016	Yes	3.069		

		trans-Cu(II)S2O2 and Cu(I)S3 cores								
72	J. Saranya, M. Sowmiya, P. Sounthari, K. Parameswari, S. Chitra and K. Senthilkumar	N-Heterocycles as corrosion inhibitors for mild steel in acid medium	J. Mol. Liq	216	42	2016	Yes	4.561		
71	M.Sowmiya and K. Senthilkumar	Adsorption of proline, hydroxyproline and glycine on anatase (001) surface - A first principle study	Theor. Chem. Acc	135	12	2016	Yes	2.233		
70	K. Navamani and K. Senthilkumar	Forth-back oscillated charge carrier motion in dynamically disordered hexathienocoronene molecules: A theoretical study	Phys. Chem. Chem. Phys	17	17729	2015	Yes	3.567		
69	K. Navamani and K. Senthilkumar	Effect of dynamic disorder on charge carrier dynamics in Ph4DP and Ph4DTP molecules	RSC Advances	5	38722	2015	Yes	3.049		
68	M.Sowmiya and K. Senthilkumar	Adsorption of RGD Tripeptide on Anatase (001) Surface - A First Principle Study	Computational Materials Science	104	124	2015	Yes	2.292		
67	M. Sethu Raman, M. Kesavan, K. Senthilkumar and V. Ponnuswamy	Ultrasonic, DFT and FT-IR studies on hydrogen bonding interactions in aqueous solutions of diethylene glycol	J. Mol. Liq	202	115	2015	Yes	4.561		
66	S. S. Bag, S. Jana, A. Yashmeen, K.	Triazolyl-donor–acceptor chromophore-decorated	Chem. Commun	50	433	2014	Yes	6.164		

	Senthilkumar and R. Bag	unnatural amino acids and peptides: FRET events in a beta-turn conformation								
65	K. Navamani and K. Senthilkumar	Effect of structural fluctuations on charge carrier dynamics in triazene based octupolar molecules	J. Phys. Chem. C	118	27754	2014	Yes	4.309		
64	R Nithya and K. Senthilkumar	Theoretical studies on the quinoidal thiophene based dyes for dye sensitized solar cell and NLO applications	Phys. Chem. Chem. Phys	16	21496	2014	Yes	3.567		
63	L Sandhiya and K. Senthilkumar	A theoretical probe on the non-covalent interactions of sulfadoxine drug with pi-acceptors	J. Mole. Str	1074	157	2014	Yes	2.120		
62	R Nithya and K. Senthilkumar	Theoretical studies on charge transport and optical properties of Tris(N-Saclicylideneanilines)	RSC Adv	4	25969	2014	Yes	3.049		
61	S. Ponnusamy, L Sandhiya and K. Senthilkumar	Mechanism and kinetics of the atmospheric degradation of perfluoropolymethylisopropyl ether by OH radical	Struct. Chem	25	1773	2014	Yes	1.624		
60	R Nithya and K. Senthilkumar	Charge transport and optical properties of cross-conjugated organic molecules: A theoretical study	Organic Electronics	15	1607	2014	Yes	3.495		

59	G. Saranya, Shiny Nair, V. Natarajan and K. Senthilkumar	Adsorption of perfluoropentacene on aluminum(100) surface: structural and electronic properties from first principle study	Computational Materials Science	89	216	2014	Yes	2.292		
58	L. Sandhiya, P. Kolandaivel and K. Senthilkumar	Oxidation and nitration of tyrosine by ozone and nitrogen dioxide – Reaction mechanisms, biological and atmospheric implications	J. Phys. Chem. B	118	3479	2014	Yes	2.923		
57	G. Saranya, K. Navamani and K. Senthilkumar	A theoretical study on optical and charge transport properties of anthra-[1,2-b:4,3-b':5,6-b'':8,7-b''']tetrathiophene molecules	Chem. Phys	433	48	2014	Yes	1.822		
56	R Nithya, M. Sowmiya, P. Kolandaivel and K. Senthilkumar	Structural, optical and charge transport properties of cyclopentadithiophene derivatives – A theoretical study	Struct. Chem	25	715	2014	Yes	1.624		
55	L. Sandhiya and K. Senthilkumar	Reaction mechanism and kinetics of the degradation of bromoxynil initiated by OH radical	RSC Adv	4	7749	2014	Yes	3.049		
54	M. Sethuram, M. Dhandapani, M.Sethu Raman, G. Amirthaganesan and K. Senthilkumar	Structure and spectral properties of L-histidinium dipicrate dihydrate	Spectrochimica Acta	118	102	2014	Yes	2.931		

53	K. Navamani, G. Saranya, P. Kolandaivel and K. Senthilkumar	Effect of structural fluctuations on charge carrier mobility in thiophene, thiazole and thiazolothiazole based oligomers	Phys. Chem. Chem. Phys	15	17947	2013	Yes	3.567		
52	G. Saranya, P. Kolandaivel and K. Senthilkumar	Opto-electronic properties of low band-gap fused ring thieno[3,4-b]pyrazine analogues - A theoretical study.	Mol. Phys	111	3036	2013	Yes	1.704		
51	L. Sandhiya, P. Kolandaivel and K. Senthilkumar	Depletion of atmospheric ozone by nitrogen dioxide: a bifurcated reaction pathway	Theor. Chem. Acc.	132	1382	2013	Yes	2.233		
50	L. Sandhiya, P. Kolandaivel and K. Senthilkumar	Mechanism and kinetics of the atmospheric oxidative degradation of dimethylphenol isomers initiated by OH radical	J. Phys. Chem. A	117	4611	2013	Yes	2.836		
49	P. Deepa, P. Kolandaivel and K. Senthilkumar	Structural properties and the effect of platinum drugs with DNA base pairs	Struct. Chem.	24	583	2013	Yes	1.624		
48	M. Muthu Tamizh, K. Senthilkumar, B.F.T. Cooper, C.L.B. Macdonald and R. Karvembu	Theoretical and experimental studies on the structure and spectroscopic properties of Ni(II) complexes of the type [Ni(L)(PPh3)] [H2L = 5-methyl-N-(2-mercaptophenyl)salicylideneimine	J. Mole. Struct.	1037	367	2013	Yes	2.210		

		and 5-chloro-N-(2-mercaptophenyl)salicylideneimine								
47	G. Saranya, Shiny Nair, V. Natarajan, P. Kolandaivel and K. Senthilkumar	A theoretical study of structural and electronic properties of Pentacene/Al(100) interface	J. Mol. Grap. Model	38	334	2012	Yes	1.863		
46	L. Sandhiya, P. Kolandaivel and K. Senthilkumar	Theoretical Studies on the reaction mechanism and kinetics of the atmospheric reactions of 1,4-thioxane with OH radical	Struct. Chem.	23	1475	2012	Yes	0.541		
45	R Nithya, P. Kolandaivel and K. Senthilkumar	Understanding the absorption and emission spectra of borondipyrromethene dye and its substituted analogs	Mol. Phys.	110	445	2012	Yes	1.704		
44	L. Sandhiya, P. Kolandaivel and K. Senthilkumar	Reaction Mechanism and kinetics of the atmospheric oxidation of 1,4-thioxane by NO_3 – A theoretical study	Can. J. Chem.	90	384	2012	Yes	1.003		
43	P. Deepa, P. Kolandaivel, K. Senthilkumar	Theoretical investigation of interaction between psoralen and altretamine with stacked DNA base pairs	Materials Science and Engineering: C	32	423	2012	Yes	4.959		
42	L. Sandhiya, P. Kolandaivel and K. Senthilkumar	Mechanism and Kinetics of the reaction of 1,4-thioxane with O_3 in the atmosphere-A theoretical Study	Chem. Phys. Lett	153	525-526	2012	Yes	1.901		

41	R. Prabhakaran, P. Kalaivani, S. V. Renukadevi, R. Huang, K. Senthilkumar, R. Karvembu and K. Natarajan	Copper ion mediated selective cleavage of C-S bond in ferrocenylthiosemicarbazone forming mixed geometrical $[(PPh_3)Cu(\mu\text{-}S)_2Cu(PPh_3)_2]$ having Cu_2S_2 core: Towards a new avenue in copper–sulfur chemistry	Inorg. Chem.	51	3525	2012	Yes	4.85		
40	G. Saranya, N. Santhanamoorthi, P. Kolandaivel and K. Senthilkumar	Charge Transport and Optical Properties of Discotic Liquid Crystalline Molecules THDDP and Substituted THDP	Int. J. Quan. Chem.,	112	713	2012	Yes	2.263		
39	G. Saranya, P. Kolandaivel and K. Senthilkumar	Optical Absorption and Emission Properties of Fluoranthene, Benzo[k]fluoranthene, and their Derivatives. A DFT Study	J. Phys. Chem. A	115	14647	2011	Yes	2.836		
38	L. Sandhiya, P. Kolandaivel and K. Senthilkumar	Reaction mechanism and kinetics of the atmospheric reactions of 2,3-dimethylphenol with OH radical	Journal of International Academy of Physical Sciences	15	359	2011	Yes	-		
37	P. Deepa , P. Kolandaivel and K. Senthilkumar	Structural Properties and the effect of interaction of alkali (Li^+, Na^+, K^+) and alkaline earth (Be^{2+}, Mg^{2+}, Ca^{2+}) metal cations with G and SG- tetrads	Comput. Theor. Chem.,	974	57-65	2011	Yes	1.403		
36	R. Nithya, N. Santhanamoorthi, P. Kolandaivel, and K. Senthilkumar	Structural and Spectral Properties of 4-Bromo-1-naphthyl Chalcones: A Quantum Chemical Study	J. Phys. Chem. A	115	6594-6602	2011	Yes	2.836		

35	N. Santhanamoorthi, K. Senthilkumar and P. Kolandaivel	Long-Range Charge Transfer in Donor-Peptide Bridge-Acceptor Model Systems - A Theoretical Study	Int. J. Qua. Chem.,	111	3904-3914	2011	Yes	2.263		
34	*P. Krishnamoorthy, P. Sathyadevi, K. Senthilkumar, P. Thomas Muthiah, R. Ramesh, N. Dharmaraj*	*Copper(I) hydrazone complexes: Synthesis, structure, DNA binding, radical scavenging and computational studies*	*Inorg. Chem. Comm.,*	14	1318-1322	2011	Yes	1.795		
33	P. Deepa , P. Kolandaivel and K. Senthilkumar	Hydrogen bonding studies of Amino acid side chains with DNA base pairs	Mol. Phys.	109	1995-2008	2011	Yes	1.704		
32	M. Karthika, K. Senthilkumar and R. Kanakaraju	Hydrogen bond interactions in hydrated acetylsalicylic acid	Comput. Theor. Chem.,	966	167-179	2011	Yes	1.403		
31	P. Deepa, P. Kolandaivel, K. Senthilkumar	First and second coordination spheres in 8-azaxanthinato salts of divalent metal aquacomplexes – Ab initio and DFT study	Polyhedron	30	1431	2011	Yes	2.284		
30	R. Shankar, P. Kolandaivel and K. Senthilkumar	A Theoretical Study on Decomposition and Rearrangement Reaction Mechanism of Trichloroacetyl Chloride (CCl3COCl)	Int. J. Qua. Chem.,	111	3482-3496	2011	Yes	2.263		
29	P. Deepa, K. Senthilkumar and P. Kolandaivel	Structural Properties and the effect of 2, 6-diaminoanthraquinone on G-tetrad, non-G-tetrads and mixed	Int. J. Qua. Chem.,	111	3239-3250	2011	Yes	2.263		

		tetrads - A density functional theory study								
28	N. Santhanamoorthi, K. Senthilkumar and P. Kolandaivel	Tautomerization and solvent effects on the absorption and emission properties of the Schiff base N,N'-bis(salicylidene)-p-phenylenediamine - A TDDFT study	Mol. Phys.	108	1817 - 1827	2010	Yes	1.704		
27	R. Shankar, P. Kolandaivel and K. Senthilkumar	Reaction mechanism of cystein proteases model compound HSH with diketone inhibitor $PhCOCOCH_{3-n}X_n$ (X= F, Cl, n= 0, 1, 2)	Int. J. Qua. Chem.,	110	1660-1674	2010	Yes	2.263		
26	N. Santhanamoorthi, K. Senthilkumar and P. Kolandaivel	Absorption and emission properties of phynelene ethynylene oligomers: Effect of substitution and π-conjugation length	Mol. Phys.	107	1629-1639	2009	Yes	1.704		
25	N. Santhanamoorthi, P. Kolandaivel and K. Senthilkumar	Effect of conformational degrees of freedom on the charge transfer in model peptides	J. Mol. Grap. Model.	27	784-791	2009	Yes	1.863		
24	Ulla Pentikainen, K. E. Shaw, K. Senthilkumar, C. J. Woods and A. J. Mulholland	Lennard-Jones parameters for B3LYP/CHARMM27 QM/MM modelling of nucleic acid bases	J. Chem. Theory Comput.,	5	396-410	2009	Yes	5.313		

23	R. Shankar, K. Senthilkumar and P. Kolandaivel	Calculation of ionization potential and chemical hardness: A comparative study of different methods.	Int. J. Quant. Chem.,	109	764-771	2009	Yes	2.263		
22	K. Senthilkumar, J. I. Mujika, K. E. Ranaghan, F. R. Manby, A. J. Mulholland and J. N. Harvey	Analysis of polarization in QM/MM modelling of biologically relevant hydrogen bonds.	*J. Roy. Soc. Interface*	5	207-216	2008	Yes	3.224		
21	P. Deepa, P. Kolandaivel and K. Senthilkumar	Interactions of anticancer drugs with usual and mismatch base pairs - Density functional theory studies.	Biophy. Chem.,	136	50-58	2008	Yes	1.745		
20	N. Santhanamoorthi, P. Kolandaivel and K. Senthilkumar	Theoretical investigation on intramolecular electron transfer in polypeptides.	Chem. Phys. Lett.,	440	302-307	2007	Yes	1.901		
19	V. Sathyabama, M. Karthika, K. Senthilkumar, K. Anandan and R. Kanakaraju	Post Hartree-Fock and density functional theory studies on di-protonated Allopurinol $^{2+}$.	J. Molec. Struct. (THEOCHEM),	810	25-30	2007	Yes	1.403		
18	N. Santhanamoorthi, P. Kolandaivel and K. Senthilkumar	Charge transfer in polypeptides: Effect of secondary structures on charge transfer integral and site–energies.	J. Phys. Chem. A,	110	11551-11556	2006	Yes	2.836		
17	S. Fratiloiu, K. Senthilkumar, F. C. Grozema, H. C- Pandya, Z. I. Niazimbetova,	Two dimensional charge delocalization in X-shaped phenylenevinylene oligomers	Chemistry of Materials,	18	2118-2129	2006	Yes	10.159		

	Y. J. Bhandari, M. E. Galvin and L. D.A. Siebbeles.									
16	K. Senthilkumar, M. Sethu Raman and P. Kolandaivel	Effect of substitution of electron-donating and -withdrawing groups on the stability of flavin-diaminepyridine complexes – A density functional theory study.	J. Molec. Struct. (THEOCHEM),	758	107-112	2006	Yes	1.403		
15	P. Prins, K. Senthilkumar, F.C. Grozema, P. Jonkneijm, A. P. H. J. Schenning, E.W. Meijer and L.D.A. Siebbeles.	Charge transport in self-organized π-stacks of p-phenylene vinylene oligomers.	J. Phys. Chem. B,	109	18267-18274	2005	Yes	2.923		
14	K. Senthilkumar, F.C. Grozema, C.F. Guerra, F.M. Bickelhaupt, F. D. Lewis, Y. A. Berlin, M. A. Ratner and L.D.A. Siebbeles.	Absolute rates of hole transfer in DNA.	J. Am. Chem. Soc.,	127	14894.	2005	Yes	14.695		
13	L. van Eijck, K. Senthilkumar, L.D.A. Siebbeles and G.J. Kearley.	A quantitative study of the charge-transfer between conjugated thiophene rings in vibrationally excited states.	Physica B,	350	220-223	2004	Yes	1.874		
12	V. Lemaur, D.A. da Silva Filho, V. Coropceanu, M. Lehmann, Y. Geerts, J. Piris,	Charge transport properties in discotic liquid crystals: A quantum-chemical insight into structure-property relationships	J. Am. Chem. Soc.,	126	3271-3279	2004	Yes	14.695		

	M.G. Debije, A.M. van de Craats, K. Senthilkumar, L.D.A Siebbeles, J.M. Warman, J.L. Brédas and J. Cornil									
11	K. Senthilkumar, F.C. Grozema, C.F. Guerra, F.M. Bickelhaupt and L.D.A. Siebbeles.	Mapping the sites for selective oxidation of guanines in DNA.	J. Am. Chem. Soc.,	125	13658-13659	2003	Yes	14.695		
10	K. Senthilkumar, F.C. Grozema, F.M. Bickelhaupt and L.D.A. Siebbeles	Charge transport in columnar stacked triphenylenes: effects of conformational fluctuations on charge transfer integrals and site-energies.	J. Chem. Phys.,	119	9809-9817	2003	Yes	2.997		
9	K. Senthilkumar and P. Kolandaivel	Structure, conformation and NMR studies on 1,2-dioxane and halogen substituted 1,2-dioxane molecules.	Computational Biology and Chemistry	27	173-183	2003	Yes	1.581		
8	K. Senthilkumar and P. Kolandaivel	Hartree-Fock and density functional theory studies on ionization and fragmentation of halomethane molecules by positron impact.	Molec. Phys.,	100	3817-3822	2002	Yes	1.704		
7	K. Senthilkumar and P. Kolandaivel	Molecular structure, conformational stability and cis effect of 1,4-dichlorobutadiene - A quantum chemical study.	J. Molec. Struct. (THEOCHEM),	577	69-79	2002	Yes	1.403		

6	K. Senthilkumar and P. Kolandaivel	Quantum chemical studies on tautomerism of barbituric acid in gas phase and in solution.	J. Comp. aided Molec. design,	16	263-272	2002	Yes	3.25		
5	K. Senthilkumar and P. Kolandaivel	Post Hartree-Fock and density functional theory studies on structure and conformational stability of nitrosoethylene and substituted compounds of nitrosoethylene.	Computers and Chemistry,	26	207-221	2002	Yes	3.334		
4	R. Kanakaraju, K. Senthilkumar and P. Kolandaivel	Origin of the cis effect – Nonbonded intr amolecular interactions: Quantum chemical studies on 1,2-dihaloethylene molecules.	J. Molec. Struct. (THEOCHEM),	589	95-102	2002	Yes	1.403		
3	K. Senthilkumar, M. Ramaswamy and P. Kolandaivel	Studies of chemical hardness and Fukui function using the exact solution of the density functional theory	Int. J. Quantum Chem.,	81	4-10	2001	Yes	2.263		
2	P. Kolandaivel and K. Senthilkumar	Ab initio and DFT studies on structure and stability of aliphatic aldoxime molecules.	J. Molec. Struct. (THEOCHEM),	535	61 - 70	2001	Yes	1.403		
1	P. Kolandaivel , N. Suba and K. Senthilkumar.	Study of chemical bonding in H_2 and HF molecule- Wave function and density functional theory (DFT) parameters approach.	Int. J. Quantum Chem.,	76	662-669	2000	Yes	2.263		

14.2 Resesarch articles in Journals (National)

S.No.	Name of the Authors	Title,	Journal name	Volume	Page Strt-End	Year	UGC CARE indexed/Not

14.3 Submission for database

S.No.	Name of the Authors	XRD/Protein/Gene/Any other	Database	ID/Ref no	Year	Papers if any

14.4 Book Publications

Sl. No.	Title of the Books /Chapters	Author	Co-Authors (s) if any	Name of the Publisher,		Month, Year	ISBN
(a) Books authored which are published by :							
International Publishers							
1	Theoretical Studies on Adsorption of Organic Molecules on Metal Surface in Computational Chemistry Methodology in	G. Saranya and K. Senthilkumar		Apple Academic Press		2017	9781771885683

	Structural Biology and Materials Sciences						
2	Theoretical Studies on mechanism and kinetics of atmospheric chemical reactions in Reaction Rate Constant Computations: Theories and Applications	L.Sandhiya and K. Senthilkumar		Royal Society of Chemistry		2013	978-1-84973-650-3
National Publishers							
Chapter in Edited Book							
Editor of Books by International Publisher							
Editor of Books by National Publisher							
(b) Translation works in Indian and Foreign Languages by qualified faculties							
Chapter or Research Paper							

Book							
					Total:	2	

15 Awards

15.1 Travel awards

S.No.	Funding agency	Name of conference	Country	Paper presented (Oral/Poster)	Title of paper	Dates
1	DST	International Congress on Quantum Chemistry 2009	Finland	Poster	Theoretical studies on absorption and emission properties of π-conjugated organic molecules	22-27 June 2009

15.2 Academic awards

S.No.	Awarding agency	Country	Purpose of award	Date of Award	Any other details
1	CSIR	India	Senior Research Fellow	November 2000	

15.3 Academic fellowships for training

S.No.	Name of faculty	Awarding agency	Institution visited	Country	Duration	Purpose	Papers if any

16 Academic events attended

16.

1 Conference /seminars /Symposium attended

S.No	Name of Authors	Title of conference	Duration	Poster /Oral/Guest speaker/Chairperson	Title of paper	Institution	Country
1	Dr. K. Senthilkumar	Theoretical Chemistry Symposium 2010 (TCS10)	5 days	Paper presented	1. Optical and conducting properties of fluoranthene and benzo (k) fluoranthene derivatives – A DFT Study 2. Theoretical studies on charge transport in thiazolothiazole, thiazole and thiophene based oligomers 3. Theoretical Studies on the atmospheric reaction of 1,4-thioxane with OH, NO3 and O3 4. Theoretical Studies on Charge Transport Properties of 2Tris(N-Saclicylideneanilines)	IIT	India
2	Dr. K. Senthilkumar	National seminar on recent advanced methods in molecular structure	2 days	Paper presented	Role of molecular vibrations in bond energy and chemical hardness.	P.S.G. College of arts and science	India
3	Dr. K. Senthilkumar	Biannual Discussion Meeting on Theoretical Chemistry	3 days	Paper presented	Post Hartree-Fock and density functional theory studies on structure and conformational stability of nitrosoethylene and	IIT	India

					substituted compounds of nitrosoethylene		
4	Dr. K. Senthilkumar	National symposium on atomic, molecular structure, interactions and Laser spectroscopy	3 days	Paper presented	Hartree-Fock and density functional theory studies on ionization and fragmentation of halomethane molecules by positron impact.	Banaras Hindu University	India
5	Dr. K. Senthilkumar	10th Annual scientific symposium on charge transport phenomena in condensed matter	1 day	-	-	Delft University of technology	The Netherlands
6	Dr. K. Senthilkumar	Lunteren meeting on structure and reactivity, Lunteren.	2 days	Paper presented	Quantum chemical calculations on charge transfer in columnar p-stacked triphenylenes.	Netherlands Organisation for Scientific Research (NWO)	The Netherlands
7	Dr. K. Senthilkumar	Sixth international symposium on functional □-electron systems	6 days	Paper presented	1. Effect of structural fluctuations on charge transport in columnar p-stacked molecules. 2. Mapping the sites for selective oxidation of guanines in DNA	Cornell University	USA
8	Dr. K. Senthilkumar	Conference on synthesis, structure and reactivity of biomolecular chemistry	3 days	Paper presented	Charge transfer in DNA hairpins: effect of structural fluctuations and Coulomb interactions	Netherlands Organisation for Scientific Research (NWO)	The Netherlands

9	Dr. K. Senthilkumar	Group symposium on molecular simulation	1 day	Paper presented	Mapping the sites for selective oxidation and charge transport in DNA	University of Heidelberg	Germany
10	Dr. K. Senthilkumar	Discussion meeting on theoretical chemistry (TCS 2009)	5 days	Paper presented	1. Theoretical studies on charge transport in π-stacked organic molecules 2. Decomposition and rearrangement reaction mechanism of trichloro acetylchloride 3. Theoretical studies on drug and DNA binding mode	Indian Institute of Science and Jawaharlal Nehru Centre for Advanced Scientific Research	India
11	Dr. K. Senthilkumar	State level workshop on introductory opto electronics	1 day	Paper presented	Molecular quantum mechanics and opto-electronics	APA Arts College for women	India
12	Dr. K. Senthilkumar	International Congress on Quantum Chemistry 2009	6 days	Paper presented	Theoretical studies on absorption and emission properties of π-conjugated organic molecules	University of Helsinki	Finland
13	Dr. K. Senthilkumar	International Symposium of Molecules and Materials (A survey of recent concepts)	2 days	Paper presented	1. Structural and spectral properties of 4-bromo-1-naphthyl chalcones - A quantum chemical study 2. Studies on charge transport in π-stacked liquid crystalline nolecules THDP and THDDP	IISER	India

					3. Theoretical studies on absorption and emission properties of π-conjugated organic molecules 4. Theoretical Study of the second coordination sphere in 8-azaxanthinato salts of divalent metal aquacomplexes		
14	Dr. K. Sethilkumar	International Conference on Applied Theory On Molecular Systems-(ATOMS 2011)	4 days	Paper presented	1. A Theoretical Study of Structural and Electronic Properties of Pentacene/Al(100) Interface 2. Theoretical studies of the oxidative degradation of dimethylphenols by OH radical in the atmosphere	IICT	India
15	Dr. K. Senthilkumar	Short term Course in Computational Methods in Chemistry	5 days	Guest speaker	Physics and Chemistry of Molecules through Quantum Mechanics	NIT	India
16	Dr. K. Senthilkumar	Symposium on Theoretical and Computational Chemistry -Frontiers and Challenges	2 days	Guest speaker	Charge Transport Properties of π-Conjugated Oligomers – A Theoretical Study	Bharathidasan University	India
17	Dr. K. Senthilkumar	Quality improvement programme in advances in new engineering materials	1 day	Guest Speaker	Physics and Chemistry of Materials through Quantum Mechanics	CIT	India

18	Dr. K. Senthilkumar	-	1 day	Guest Speaker	Application of DFT to Find and Tune the Suitable Materials for Solar Energy Applications	Beijing computational science research center	China
19	Dr. K. Senthilkumar	National workshop on Programming for data analytics	3 days	Guest Speaker	Programming with ForTran	TNAU	India
20	Dr.K. Senthilkumar	State Level Symposium on Spectroscopic Perspective of Quantum Dots	1 day	Guest speaker	An overview of Molecular Quantum Mechanics and its Applications in Opto-Electronics	Govt. Arts College for Women	India
21	Dr.K. Senthilkumar	National Symposium on Recent Advances in Chemistry	1 day	Guest speaker	An Overview of Molecular Quantum Mechanics and its Application to Model Atmospheric Chemical Reactions	Dept. of Chemistry, Pondicherry University	India

16.2 Workshop/Training/FDP attended

S.No	Title	Duration	Institution	Country
1	Workshop on preparation of project proposals for funding and research publications, organized by Research and Development Cell.	20.09.2008	Bharathiar University	India
2	Faculty Orientation on internal quality assurance, organized by Internal quality assurance cell (IQAC)	15.10.2008	Bharathiar University	India
3	Participated in 73rd Orientation course organized by UGC-Academic Staff College	04.02.09 to 03.03.09	Bharathiar University	India
4	Participated in Refresher course in theoretical physics organized by Indian Academy of Sciences, Bangalore and Department of Physics, Bishop Moore College	7.12.2009 to 19.12.2009	Bishop Moore College	India
5	Participated in Refresher course in physics organized by UGC-Academic Staff College	09.06.11 to 29.0.611	Bharathiar University	India

6	Participated in Refresher course in physics organized by UGC-Academic Staff College	11.09.2013 to 01.10.2013	Bharathiar University	India
7	Participated in Short Term Course on Teaching and Learning Techniques in Higher Education conducted at UGC-Human Resource Development Centre (HRDC)	29.08.2016 to 03.09.2016	Bharathiar University	India

17 Events Organized

S. No.	Title of the Event	Duration	Funding agency	Role	No. of Institutions	No. of days	No. of Institutions from other state	No. of participants	No. of experts
	Workshop on theoretical physics	19th to 22nd December 2011		Organizer	25	4	---	50	4
1	Workshop on theoretical physics	17th to 20th December 2012		Organizer	22	4	---	60	4
2	Workshop on theoretical physics	09th-12th December, 2013		Organizer	20	4	---	70	4
3	Refresher course in physics	3rd to 23rd December 2014	ASC - BU	Organizer	25	20	3	28	30

1

8 Invited and Guest Lectures Delivered in Various Capacities

S. No.	Name of the Event	Title	Institution	Date	Role
1	National Symposium on Recent Advances in Chemistry	An Overview of Molecular Quantum Mechanics and its Application to Model Atmospheric Chemical Reactions	Dept. of Chemistry, Pondicherry University	19.02.2020	Invited Lecture
1	State Level Symposium on Spectroscopic Perspective of Quantum Dots	An overview of Molecular Quantum Mechanics and its Applications in Opto-Electronics	Govt. Arts College for Women, Salem	23rd September 2019	Invited Lecture
2	National workshop on Programming for data analytics	Programming with ForTran	Tamil Nadu Agricultural University, Coimbatore	1st, 2nd and 5th August 2019	Invited Lecture
3	Beijing computational science research	Application of DFT to Find and Tune the Suitable Materials for Solar Energy Applications	Beijing computational science research center, Beijing, China	14 th June 2017	Invited Lecture
4	Quality improvement programme in advances in new engineering materials	Physics and Chemistry of Materials through Quantum Mechanics	Coimbatore institute of Technology, Coimbatore	26 November 2015	Invited Lecturer
5	Symposium on Theoretical and Computational Chemistry -Frontiers and Challenges	Charge Transport Properties of π-Conjugated Oligomers – A Theoretical Study	Bharathidasan University, Tiruchirappalli	14-15 June 2013	Invited Lecturer
6	Short term Course in Computational Methods in Chemistry	Physics and Chemistry of Molecules through Quantum Mechanics	National Institute of Technology, Tiruchirappalli	23-27 July 2012	Invited Lecturer

19 Extension activity (Social activity/election duty/special duty)

S.No.	Name of faculty	Nature of duty	Duration	Place of activity	Any other detail