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Education

Degree	University/Institute	Details	Year
Ph.D	Indian Institute of Technology Kanpur	Thesis Title: Atoms and Molecules in a Confined Environment Supervisor: Prof. N. Sathyamurthy	2008
M. Phil	University of Calicut	Thesis Title: A Preliminary Theoretical Investigation of Cation- π Interaction Supervisor: Prof. M. P. Kannan	2002
M.Sc	University of Calicut	First Class	1999

Teaching Experience

Position	University/Institute	Year
Assistant Professor	Indian Institute of Technology Roorkee	November 2012-
Assistant Professor (Contractual)	Indira Gandhi National Tribal University, Amarkantak	September 2011 – January 2012
Guest Lecturer	Zamorin's Guruvayurappan College, Calicut, Kerala	September 2002- March 2003
Guest Lecturer	Govt. College Kasaragod, Kerala	June 2000 – March 2001
Guest Lecturer	Govt. College Kasaragod, Kerala	January 2000- March 2000

Post Doctoral Research Experience

Position	University/Institute	Supervisor	Year
Post Doctoral Research Associate	Faculty of Science University of Ontario Institute of Technology (UOIT), Canada	Prof. Fedor Y. Naumkin	2012 May- 2012 November
Post Doctoral Research Associate	Department of Chemical and Biological Engineering, The State University of New York at Buffalo, USA	Prof. Eli Ruckenstein	2009 March- 2011 March
Project Scientist	Department of Chemistry Indian Institute of Technology Kanpur	Prof. N. Sathyamurthy	2008 December-2009 March
Post Doctoral Research Associate	Department of Chemistry University of Perugia, Italy	Prof. Vincenzo Aquilanti	2007 November-2008 November

Research Projects

No.	Title of the Project	Funding Agency	Amount (Lakhs)	Status
1.	Computational Designing of Stimuli Responsive Complexes Based on Carbon Nanostructures	SERB	42.35	2018-2021 (In progress)
2	Structure, Stability And Properties of Carbon Intercalated Gold, Palladium And Platinum Clusters	CSIR	6.00	2017-2020 (In progress)
3.	Formation, Structure, Stability And Thermodynamic Properties of Mixed Gas Hydrates	SERB	28.73	2013-2016 (Completed)
4	Effect of Cage Substitution And Endohedral Doping on Alignment And Properties of Fullerenes And Carbon Nanotubes	IIT Roorkee	8.83	2013-2016 (Completed)

Research Supervision

Degree	Ph.D Thesis Completed/Submitted	In Progress	Total
Ph.D	2 Completed	5	7
M.Tech	4 completed	1	5
M.Sc	4 completed	1	5

Details of Thesis Supervised

Degree	Name of the Student	Title of the Thesis	Status
Ph.D	1. Ms. Surinder Pal Kaur	Computational Studies of Selected Gas Hydrates and Hydrate Melts	Completed
	2. Mr. Sujith K. S	Molecular Dynamics Studies of Mixed Gas Hydrate Melts and Aqueous Interfaces	Completed
	3. Ms. Ankita Joshi	Structure and Properties of π - π Interacting Complexes of Carbon Nanotubes	In Progress
	4. Mr. Vinit.	Computational Studies of the Derivatives of Fullerenes and Carbon Nanotubes	In Progress
	5. Mr. Mohan Tiwari	Computational Studies of Structure, Stability and Properties of Carbon Intercalated Gold Clusters	In Progress
	6. Mr. Angat Dhiman	Studies on stimuli responsive complexes based on carbon nanostructures	In Progress
	7. Mr. Peaush Gangwar	Catalytic reduction of CO ₂ using selected metal complexes	In Progress
M.Tech	1. Mr. V. Shilpi	Structural Pattern and the Stability of Water Clusters in Gas Hydrates	Completed
	2. Ms. Bhawana Singh Tomar	Promoters and Inhibitors of Gas Hydrates	Completed
	3. Ms. Suman Lata	Clustering of Some Atmospherically Important Molecules: A Computational Study	Completed
	4. Mr. Rajdeep Shehrawat	Interaction of Carbon Nanotube with Tau Protein: A Molecular Dynamics Simulation Based Study	Completed
	5. Mr. Rajat Pundhir	Effect of roughness of interface on the dissolution of gas molecules: The case of CO ₂	In Progress
M. Sc	1. Ms. Sakshi Ganotra	Interaction of Endosulfan with Flat and Curved Carbon Surfaces	Completed
	2. Ms. Manisha Prakashni	Structure and Optical Properties of Oxadiazole and its Derivatives: A Computational Study	Completed
	3. Mr. Mohit Rohilla	A Computational Study of Interaction Between Natural Collagen of Type-I and Carbon Nanotube	Completed
	4. Mr. Laukesh Kr. Sharma	A Preliminary Theoretical Study of Pd _n C _m ($n, m = 1-5$) Clusters	Completed
	5. Mr. Vishal Kumar Yadav	Density functional studies of PKa values of Selected Compounds	In Progress

Research Papers Published in Journals (Summary)

Details	ACS	RSC	Elsevier	Wiley	Taylor& Francis	Springer	Total
After Joining IIT Roorkee (2013-)	5	7	9	0	1	0	22 + 4 submitted
Before Joining (2003-2012)	4	0	6	1	0	3	14
Total	9	6	15	1	1	3	36 + 4 submitted

PUBLICATIONS

Sl. No	Authors	Title of the paper	Year, Volume, Page	Journal
1	A. Joshi, C. N. Ramachandran	High-bias Negative Differential Resistance Effect in Pure, Doped and Co-Doped Carbon Nanotubes Connected to Boron Nitride Nanotubes	Manuscript Submitted	
2	A. Joshi, C. N. Ramachandran	Optoelectronic and Charge Transport Properties of the Donor-Acceptor Complex of Carbon Nanotube with Perylene Bisimide	Manuscript Submitted	
3	M. Tiwari, Vinit, C. N. Ramachandran	Catalytic reduction of SO ₂ by CO using carbon intercalated gold clusters	Manuscript Submitted	
4	M. Chaudhary, R. Muhammad, C. N. Ramachandran, P. Mohanty	Nitrogen Amelioration Driven Carbon Dioxide Capture by Nanoporous Polytriazine	Manuscript Submitted	
5	Vinit, C. N. Ramachandran	Spin Density Transfer from Guest to Host in Doped And Substituted Fullerenes	2019, in press	Phys. Chem. Chem. Phys.
6	A. Joshi, C. N. Ramachandran	Structure, Stability and Optoelectronic Properties of Cycloparaphenylene-Carbon Nanotube based molecular architectures	2018,122, 19904-19912	J.Phys. Chem. C
7	S.P. Kaur, C. N. Ramachandran	Structure, Stability and NMR Chemical Shifts of Hydrogen-Tetrahydrofuran Mixed Hydrates: A Computational Study	2018,43, 19559-19566	Int. J. Hydr. Energy

8	K. S. Sujith, C. N. Ramachandran	Effect of surface roughness on distribution of gas molecules adsorbed on the water-methane interface	2018 ,266, 856-863.	J. Mol. Liquids
9	K. S. Sujith, Km. Suman Lata, C. N. Ramachandran	Adsorption and Dissolution of Methane at the Surface of the Methanol-Water Mixture	2018 ,473, 310-317.	Fluid Phase Equilibria
10	A. Joshi, C. N. Ramachandran	Structural, Optoelectronic and Charge Transport Properties of the Complexes of Indigo Encapsulated in Carbon Nanotubes	2018 ,20, 15158-15167	<i>Phys. Chem. Chem. Phys.</i>
11	R. Kumar, H. Jain, P. Gahlyan, A. Joshi, C. N. Ramachandran	A highly sensitive pyridine-dicarbohydrazide based chemosensor for colorimetric recognition of Cu^{2+} , AMP^{2-} , F^- and AcO^- ions	2018 , 42, 8567-8576	<i>New J. Chem</i>
12	S. P. Kaur, K. S. Sujith, C. N. Ramachandran	Formation of Nanobubble and its Effect on the Structural Ordering of Water in $\text{CH}_4\text{-N}_2\text{-CO}_2\text{-H}_2\text{O}$ Mixture	2018 , 20, 9157-9166	<i>Phys. Chem. Chem. Phys.</i>
13	S. P. Kaur, C. N. Ramachandran	Host-Guest and Guest-Guest Interactions in Noble Gas Hydrates	2018 , 1, 54-63	<i>Mol. Phys.</i>
14	A. Joshi, C. N. Ramachandran	A Comprehensive Study of the Optoelectronic Properties of Donor-Acceptor Based Derivatives of 1,3,4-Oxadiazole	2017 , 679, 102-111	<i>Chem. Phys. Lett.</i>
15	A. P. Sivadas, D. S. S. Rao, N. S. S. Kumar, D. D. Prabhu, S. Varghese, C. N. Ramachandran, R. M. Ongungal, S. K. Prasad, Suresh Das	Self-Assembling and Luminescent Properties of Chiral Bis-oxadiazole Derivatives in Solution and Liquid Crystalline Phases.	2017 , 121, 1922-1929	<i>J. Phys. Chem. B.</i>
16	Vinit, C. N. Ramachandran	Structure, stability and properties of boron encapsulated complexes of C_{60} , C_{59}B and C_{59}N .	2017 , 121, 1708-1714	<i>J. Phys. Chem. A</i>
17	K. S. Sujith, C. N. Ramachandran	Natural gas evolution in a gas hydrate melt: Effect of thermodynamic hydrate inhibitors.	2017 , 121, 153-163	<i>J. Phys. Chem. B</i>
18	Vinit, K. S. Sujith, C. N. Ramachandran	Spin-spin coupling in nitrogen atom encapsulated C_{60} , C_{59}N and their respective dimmers.	2016 , 120, 6990-6997.	<i>J. Phys. Chem. A.</i>

19	M. Prakashni, A. Joshi, C. N. Ramachandran	Electronic and optical absorption properties of the derivatives of 1,3,4-oxadiazole	2016,5/6, 88-95.	<i>Chemical Data Collections</i>
20	S. P. Kaur, C. N. Ramachandran	Effect of multiple and adjacent cage occupancies on host-guest interaction and NMR chemical shifts in gas hydrates	2016, 1092, 57-67	<i>Comp. Theor. Chem.</i>
21	A. Joshi, C. N. Ramachandran	Charge transport and optical properties of the complexes of indigo wrapped over carbon nano tubes	2016, 18, 14040-14045	<i>Phys. Chem. Chem. Phys.</i>
22	K. S. Sujith, C. N. Ramachandran	Carbon dioxide induced bubble formation in a CH ₄ -CO ₂ -H ₂ O ternary system: A molecular simulation study	2016, 18, 3746-3754.	<i>Phys. Chem. Chem. Phys.</i>
23	V. Shilpi, S. P. Kaur, C. N. Ramachandran	Density functional studies of fused dodecahedral and irregular dodecahedral cages	2015,5, 74270-74273	<i>RSC Advances</i>
24	V. Shilpi, S.P. Kaur, C.N. Ramachandran	Revisiting the structural pattern and the stability of (H ₂ O) ₂₀ clusters using the dispersion corrected density functional method	2015, 626, 39-42.	<i>Chem. Phys. Lett.</i>
25	P. Kumar, B. K. Mishra, C. N. Ramachandran, N.Sathyamurthy	Interaction of rare gas dimers in the confines of a carbon nanotube	2015, 618, 42-45.	<i>Chem. Phys. Lett.</i>
26	A. Equbal, S. Srinivasan, C.N. Ramachandran, N. Sathyamurthy	Encapsulation of paramagnetic diatomic molecules B ₂ , O ₂ and Ge ₂ inside C ₆₀	2014,610-611, 251-255	<i>Chem. Phys. Lett.</i>
Before Joining IIT Roorkee				
27	C. N. Ramachandran, F. Y Naumkin	Structure and properties of small aurocarbons: a selective study	2013, 117, 6803-6808	<i>J. Phys. Chem. A</i>
28	C. N. Ramachandran, B. K. Mishra, A. K. Tiwari	Density functional studies of endosulfan and its interaction with glycine and GABA	2012,124, 203-207	<i>J. Chem.Sci,</i>
29	C. N. Ramachandran, Eli Ruckenstein	Encapsulation of interstellar abundant H ₃ ⁺ in a C ₆₀ fullerene	2011,111, 3695-3700.	<i>Int.J.Quant.Chem.</i>
30	C. N. Ramachandran, Eli Ruckenstein	Density functional theoretical studies of the isomers of croconic acid and their dimers	2011,973, 28-32	<i>Comp. Theor. Chem.</i>

31	C. N. Ramachandran, Eli Ruckenstein	Water Clustering around CO ₂ molecule	2011,966, 84-90.	<i>Comp. Theor. Chem.,</i>
32	C. N. Ramachandran, D. De Fazio, N. Sathyamurthy, V. Aquilanti	Guest species trapped in carbon nanotubes	2009, 473, 146-150	<i>Chem. Phys. Lett.</i>
33	C. N. Ramachandran, D. De Fazio, S. Cavalli, F. Tarantelli, V. Aquilanti	Revisiting the potential energy surface for the He + H ₂ ⁺ → HeH ⁺ + H reaction at the full configuration interaction level	2009, 469, 26-30	<i>Chem. Phys. Lett.,</i>
34	C. N. Ramachandran, D. Roy, N. Sathyamurthy	Host-guest interactions in endohedral fullerenes	2008, 461, 87-92.	<i>Chem. Phys. Lett.</i>
35	C. N. Ramachandran, N. Sathyamurthy	A Time-Dependent Density Functional Theoretical Study of BN-Substituted C ₆₀	2007,111, 6901-6903	<i>J. Phys. Chem. A.</i>
36	C. N. Ramachandran, N. Sathyamurthy	Introducing a twist in carbon nanotube	2006, 91 1503-1505	<i>Curr. Science.,</i>
37	O. Shameema, C. N. Ramachandran, N. Sathyamurthy	Blue shift in X-H stretching frequency of molecules due to confinement	2006,110, 2-4	<i>J. Phys. Chem. A,</i>
38	Elango, R. Parthasarathi, V. Subramanian, C. N. Ramachandran, N. Sathyamurthy	Hydrogen peroxide clusters: The role of open book motif in cage and helical structures	2006,110, 6294-6300	<i>J. Phys. Chem. A,</i>
39	M. Elango, R. Parthasarathi, V. Subramanian, C. N. Ramachandran, N. Sathyamurthy	Atomic and molecular clusters: designer materials for the nanoworld	2005,71, 405-410	<i>Proc. Indian Natn. Sci. Acad., Part-A</i>
40	C. N. Ramachandran, N. Sathyamurthy	Water clusters in a confined nonpolar environment	2005, 410,348-351.	<i>Chem. Phys. Lett.</i>

Book chapter

1. Germanium encaged fullerene-synthesis, extraction, theoretical calculation and their possible application
Debmalya Roy, B. Shastria, C. N. Ramachandran, B. K. Mishra, K. Mukhopadhyay, N. Sathyamurthy and K. U. Bhaskar Rao
Book: Germanium: Properties, Production and Applications
Editor: Regina V. Germano
2011 Nova Science Publishers, Inc., New York

Recent Seminars/conferences/Institutes visited

No	Name of the conference	Institute	Participation/presentation	Date
1.	Advanced Simulation Methods	IIT Delhi	Presentation	8-10 March, 2019
2.	Theoretical Chemistry Symposium (TCS-2018)	BITS Pilani	Presentation	13-16 February, 2019
3	International Conference on Physics and Chemistry of Materials (ICCPM-2019)	St. Thomas College, Thrissur, Kerala	Presentation	19-21 December, 2018
4	National Seminar on Material Science and Technology for Sustainable Future	Malabar Christian College , Calicut, Kerala	Presentation	18 December, 2018
5	Institute Visit	IIT Ropar	Presentation	10 July, 2018
6	North West Meeting on Spectroscopy, Structure and Dynamics (SDD-2018)	MNIT Jaipur	Presentation	16-18 March, 2018
7	Spectroscopy, Dynamics and Molecular Clusters (SDMC-2018)	IISER Kolkata, SINP Kolkata, IACS Kolkata	Presentation	14-18 February, 2018
8	8 th Asia Pacific Conference on Theoretical and Computational Chemistry	Indian Institute of Technology Bombay	Presentation	14-17 December, 2017
9	Workshop on Computational Chemistry	Institute for Integrated Programmes and Research in Basic Sciences, M.G. University, Kottayam, Kerala	Lecture and practical session	22 June, 2017
10	North West Meeting on Structure, Spectroscopy and Dynamics	BITS Pilani	Presentation	20-22 February, 2017
11	Theoretical Chemistry Symposium	Hyderabad Central University, ICT Hyderabad, IIT Hyderabad	Participation	13-17 December, 2016
12	JSPS-DST Asian Academic Seminar	IACS Kolkata & IISER Kolkata	Participation	6-10 March, 2015
13	Theoretical Chemistry Symposium	NCL Pune & IISER Pune	Participation	18-21 December, 2014

Teaching (UG/PG Courses)

Sl. No	Course Code	Course Title	Program	Year/ Semester
1	CYN-103	Computer Programming	Int. Msc. -(1 st year)	2018-19/A
2	CYN-501	Quantum Mechanics, Symmetry and Group Theory	M.Sc-1 st year	2018-19/A
3	CYN-741	Chemometrics and Modeling	M.Tech & Pre-Ph.D	2018-19/A
4	CYN-104	Physical Chemistry-I	Int. M.Sc -1 st year	2017-18/S
5	CYN-504	Kinetics & Photochemistry	M.Sc-1 st year	2016-17/S
6	CYN-782	Chemistry of Industrial Processes	M.Tech & Pre-Ph.D	2017-18/S
7	CYN-103	Computer Programming	Int. Msc. -(1 st year)	2017-18/A
8	CYN-501	Quantum Mechanics, Symmetry and Group Theory	M.Sc-1 st year/ Int.M.Sc-4 th year	2017-18/A
9	CYN-741	Chemometrics and Modeling	M.Tech & Pre-Ph.D	2017-18/A
10	CYN-504	Kinetics and Photochemistry	M.Sc-1 st year	2016-17/S
11	CYN-782	Chemistry of Industrial Processes	M.Tech & Pre-Ph.D	2016-17/S
12	CYN-501	Quantum Mechanics, Symmetry and Group Theory	M.Sc-1 st year/ Int.M.Sc-4 th year	2016-17/A
13	CYN-741	Chemometrics and Modeling	M.Tech & Pre-Ph.D	2016-17/A
14	CYN-504	Kinetics and Photochemistry	M.Sc-I year Int. M.Sc-4 th year	2015-16/S
15	CYN-782	Chemistry of Industrial Processes	M.Tech & Pre-Ph.D	2015-16/S
16	CY-001	Physical Chemistry-I	B.Tech	2015-16/A
17	CYN-501	Quantum Mechanics, Symmetry and Group Theory	M.Sc-I year/ Int.M.Sc-4 th year	2015-16/A
18	CYN-741	Chemometrics and Modeling	M.Tech & Pre-Ph.D	2015-16/A
19	CY-332	Nuclear and Radio Chemistry	Int. M.Sc-3 rd year	2014-15/S
20	CYN-782	Chemistry of Industrial Processes	M.Tech & Pre-Ph.D	2014-15/S
21	CY-001	Physical Chemistry-I	B.Tech	2014-15/A
22	CY-331	Physical Chemistry-II	Int. M.Sc-3 rd year	2014-15/A
23	CY-511	Quantum Mechanics, Symmetry and Group Theory	M.Sc-1 st Year/	2014-15/A

			Int. M.Sc 4 th year	
24	CY-741	Chemometrics and Modeling	M.Tech & Pre-Ph.D	2014-15/A
25	ICY-03	Introduction to Photochemistry	B. Tech (Inst. Elective)	2013-14/S
26	CY-001	Physical Chemistry-I	B.Tech	2013-14/A
27	CY-511	Quantum Mechanics, Symmetry and Group Theory	M.Sc-1 st year/ Int. M.Sc 4 th year	2013-14/A
28	CY-637	Advanced Physical Chemistry-I	M.Sc-2 nd Year	2013-14/A
29	CY-722	Chemometrics and Modeling	M.Tech & Pre-Ph.D	2012-13/S
30	CY-752	Analysis of Food and Drugs	M.Tech & Pre-Ph.D	2012-13/S

Courses Developed

No.	Details of the Course	Program
1.	CYN-103: Computer Programming	Int. M.Sc
2.	CYN-515: Art of Scientific and Technical Writing	Int. M.Sc
3.	CYN-610: Molecular Modeling and Simulations	M.Sc

Contribution to Curriculum Development

No.	Details of the Course	Program
1.	CYN-101: Introduction to Chemical Sciences	Int. M.Sc
2.	CYN-102: Physical Chemistry-I	Int. M.Sc
3.	CYN-301: Quantum Chemistry and Chemical Bonding	Int. M.Sc
4.	CYN-302: Group Theory and Spectroscopy	Int. M.Sc
5.	CYN-501: Quantum Chemistry, Group Theory and Symmetry	M.Sc
6.	CYN-504: Kinetics and Photochemistry	M.Sc
7.	CYN-510: Laboratory-II	M.Sc
8.	CYN-511: Laboratory-I	M.Sc
9.	CYN- 629: Advanced Physical Chemistry	M.Sc

Responsibilities at Institute and Department Levels

No.	Administrative Responsibilities	Year
1	Member, Institute Research Committee, IIT Roorkee	2014 -2018
2	Member, Advisory Board, Continuing Education Centre, IIT Roorkee	2015-
3	Deputy Chief Advisor, Cinema Club, IIT Roorkee	2014-2017
4	Dept. Representative, ERP, IIT Roorkee	2015-
5	Member, Review Committee for Ph.D Admission Process	2018
6	Member, Review Committee for External Ph.D Supervision	2018
7	Convener, Department Faculty Search Committee, Chemistry, IITR	2014-2016
8	In Charge, Department Research Committee, Chemistry, IITR	2015-2018
9	In Charge, Chemistry Association, IITR	2014-
10	Member, Department Administrative Committee, Chemistry, IITR	2016-2018
11	Member, Student Research Committees, Chemistry and Physics, IITR	2013-
12	Joint Secretary, International Conference on Advanced Materials for Energy, Environment and Health (ICAM-2016)	2016

Conferences Organized/Organizing

Convener, 3rd North West Meeting on Structure, Spectroscopy and Dynamics (SSD-2019), 5-7 April, 2019

Joint Secretary-International Conference on Advanced Materials for Energy, Environment and Health (ICAM-2016)

Other Scientific Activities

Reviewer: Journal of Chemical Physics, J. Physical Chemistry A/B/C, Langmuir, Chemical Communications, Physical Chemistry Chemical Physics, RSC Advances, New Journal of Chemistry, Advanced Material Chemistry A, Material Chemistry-C, Chemical Physics, Scientific Reports, International Journal of Quantum Chemistry, Journal of Chemical Sciences, Current Science, Molecular Structure, AIP Advances, Chemistry Select, Chemical Reaction Intermediates, Chemical Data Collections.

Awards/Fellowships

1. Biography selected in the 2010 edition of Marquis Who's who in the world.
2. Fellowship from the Research Foundation, State University of New York
3. Fellowship from the Italian Ministry of University and Research
4. Cleared National Eligibility Test with Research Fellowships
5. Sree Guruvayurappan Scholarship for the Best Student in B.Sc Chemistry, Sree Krishna College Guruvayur, Kerala