

## Dr. RAMACHANDRAN C. N.

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<https://iitr.ac.in/Departments/Chemistry%20Department/People/Faculty/100604.html>

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### Teaching Experience

Position	University/Institute	Year
Associate Professor	Indian Institute of Technology Roorkee	December 2019-
Assistant Professor	Indian Institute of Technology Roorkee	November 2012-November 2019
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

## 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- $\pi$ Interaction Supervisor: Prof. M. P. Kannan	2002
M.Sc	University of Calicut	First Class	1999

## 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	2018-2022
2	Structure, Stability and Properties of Carbon Intercalated Gold, Palladium and Platinum Clusters	CSIR	6.00	2017-2020
3.	Formation, Structure, Stability and Thermodynamic Properties of Mixed Gas Hydrates	SERB	28.73	2013-2016
4	Effect of Cage Substitution and Endohedral Doping on Alignment and Properties of Fullerenes and Carbon Nanotubes	IIT Roorkee	8.83	2013-2016

### Research Papers Published

Sl. No	Authors	Title of the paper	Year, Volume, Page	Journal
59.	A. Hadiya, P. Gangwar, P. Sajith, C. N. Ramachandran	Probing the Interaction of NO with C <sub>60</sub> : Comparison between Endohedral and Exohedral Complexes	<a href="https://doi.org/10.1021/acs.jpca.3c00381">https://doi.org/10.1021/acs.jpca.3c00381</a>	<i>J. Phys. Chem. A</i>
58.	A. Poddar, C. N. Ramachandran, P. K. Chattaraj,	Behavior of HF and (HF) <sub>2</sub> inside a fullerene cage: An in silico study using different density functionals	2022, 123,27067	<i>Int. J. Quant. Chem.,</i>
57.	A. Dhiman, C. N. Ramachandran,	Opto-electronic properties of isomers of azobispyridine	2022, 805, 139956	<i>Chem. Phys. Lett.,</i>
56.	P. Gangwar, S.S. Negi, V. Ramanathan, C. N. Ramachandran,	Effect of confinement on the electronic and optical properties of azobenzene: cucurbituril as a means of confinement	2022, 120,2109523	<i>Mol. Phys.</i>
55.	Paras, A. Dhiman, C. N. Ramachandran	Effect of aromatic linkers on thermally activated delayed fluorescence of selected organic molecules	2022, 801,139711	<i>Chem. Phys. Lett.</i>
54.	M. Tiwari, C. N. Ramachandran	Clustering of Auro-acetylenes via C-Au... pi Interactions: Gold- Hydrogen Analogy	2022,793,139387	<i>Chem. Phys. Lett.</i>
53.	A. Dhiman, C. N. Ramachandran	Cis–trans isomerisation and absorption properties of the ring-extended azobenzene	2021, 119, 23	<i>Mol. Phys.</i>
52.	V. Aquilanti, H. E. Montgomery, C. N. Ramachandran, N. Sathyamurthy	Atoms and molecules in a confined environment (Editorial)	2021,75,1	<i>Eur. Phy. J. D.</i>
51.	P Gangwar, M Tiwari, A Narwal, CN Ramachandran	Density functional studies on the conversion of hydrogen cyanide to vinyl isocyanide using carbon-supported platinum catalysts	2021, 1205, 113442	<i>Comp. Theor. Chem.</i>
50.	Anshul Aggarwal, Paras, C. N. Ramachandran	Stacked dimers of Fe-porphyrin with hydrazine and pyrazine as Linkers	2021,779, 138826	<i>Chem. Phys.Lett.</i>
49.	P. Gangwar, P. K. Sajith, C. N. Ramachandran	Clustering of carbon dioxide around zinc oxide clusters,	2021, 771,138499	<i>Chem. Phys. Lett.</i>

48.	M. Tiwari, C. N. Ramachandran	Density functional studies of the catalytic oxidation of CO using small aurocarbons	2021, 2, 100023	<i>Chem. Phys. Impact</i>
47.	M. Tiwari, C. N. Ramachandran	Hydracyanation of acetylene on carbon intercalated gold clusters: Co-operativity and site specificity,	2020, 761, 138059	<i>Chem. Phys. Lett.</i>
46.	R. Sharma, A. Bansal, C.N.Ramachandran, P. Mohanty	A multifunctional triazine-based nanoporous polymer as a versatile organocatalyst for CO <sub>2</sub> utilization and C–C bond formation	2019, 55,11607-11610	<i>Chem. Comm.</i>
45	A. Joshi, C. N. Ramachandran	Switching the charge transfer characteristics of quaterthiophene from p-type to n-type via interactions with carbon nanotubes	2019, 21, 24820-24827	<i>Phys. Chem. Chem. Phys.</i>
44	H. Jain, N. Deswal, A. Joshi, C. N. Ramachandran, R.Kumar	Triazole-appended pyrano [2,3-c] pyrazolone based colorimetric chemosensors for recognition of Fe <sup>3+</sup> ions and their molecular logic gate behavior	2019, 11, 3230-3243	<i>Anal. Meth.</i>
43	H. Jain, A. Joshi, C. N. Ramachandran, R. Kumar	Synthesis of a Highly Efficient Multifunctional Copper (II)-Pyridyl Complex for Adsorption and Photocatalytic Degradation of Organic Dyes	2019, 4 (17), 4952-4961	<i>Chem. Sel.</i>
42	P. Gahlyan, R. Bawa, H. Jain, M. Dalela, A. Joshi, C. N. Ramachandran	Isatin-Triazole-Functionalized Rhodamine: A Dual Sensor for Cu <sub>2</sub> <sup>+</sup> and Fe <sub>3</sub> <sup>+</sup> Ions and Its Application to Cell Imaging	2019, 4 (25), 7532-7540	<i>Chem. Sel.</i>
41	P. R. Remya, B. K. Mishra, C. N. Ramachandran, N. Sathyamurthy	Effect of confinement on structure, energy and vibrational spectra of (HF) n, n= 1–4	2019, 733, 136670	<i>Chem. Phys. Lett.</i>
40	A. Joshi, C. N. Ramachandran	High-bias Negative Differential Resistance Effect in Pure, Doped and Co-Doped Carbon Nanotubes Connected to Boron Nitride Nanotubes	2019,113, 1-7	<i>Physica E: Low-dimensional Systems and Nanostructures</i>
39	A. Joshi, C. N. Ramachandran	Optoelectronic and Charge Transport Properties of the Donor-Acceptor Complex of Carbon Nanotube with Perylene Bisimide	2019, 119 (24), e26026	<i>Int. J. Quantum. Chem.</i>
38	M. Tiwari, Vinit, C. N. Ramachandran	Catalytic reduction of SO <sub>2</sub> by CO using carbon intercalated gold clusters	2019,726,111-116	<i>Chem. Phys. Lett.</i>
37	M. Chaudhary, R. Muhammad,	Nitrogen Amelioration Driven Carbon Dioxide Capture by Nanoporous Polytriazine	2019,35, 4893-4901	<i>Langmuir</i>

	C. N. Ramachandran, P. Mohanty			
36	Vinit, C. N. Ramachandran	Spin Density Transfer from Guest to Host in Doped and Substituted Fullerenes	2019,21,7605-7612	<i>Phys. Chem. Chem. Phys.</i>
35	A. Joshi, C. N. Ramachandran	Structure, Stability and Optoelectronic Properties of Cycloparaphenylene-Carbon Nanotube based molecular architectures	2018,122,19904-19912	<i>J.Phys. Chem. C</i>
34	S.P. Kaur, C. N. Ramachandran	Structure, Stability and NMR Chemical Shifts of Hydrogen-Tetrahydrofuran Mixed Hydrates: A Computational Study	2018,43, 19559-19566	<i>Int. J. Hydr. Energy</i>
33	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.	<i>J. Mol. Liquids</i>
32	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.	<i>Fluid Phase Equilibria</i>
31	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>
30	R. Kumar, H. Jain, P. Gahlyan, A. Joshi, C. N. Ramachandran	A highly sensitive pyridine-dicarbohydrazide based chemosensor for colorimetric recognition of Cu <sup>2+</sup> , AMP <sup>2-</sup> , F <sup>-</sup> and AcO <sup>-</sup> ions	2018, 42, 8567-8576	<i>New J. Chem</i>
29	S. P. Kaur, K. S. Sujith, C. N. Ramachandran	Formation of Nanobubble and its Effect on the Structural Ordering of Water in CH <sub>4</sub> -N <sub>2</sub> -CO <sub>2</sub> -H <sub>2</sub> O Mixture	2018, 20, 9157-9166	<i>Phys. Chem. Chem. Phys.</i>
28	S. P. Kaur, C. N. Ramachandran	Host-Guest and Guest-Guest Interactions in Noble Gas Hydrates	2018, 1, 54-63	<i>Mol. Phys.</i>
27	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>
26	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>

25	Vinit, C. N. Ramachandran	Structure, stability and properties of boron encapsulated complexes of C <sub>60</sub> , C <sub>59</sub> B and C <sub>59</sub> N.	2017, 121, 1708-1714	<i>J. Phys. Chem. A</i>
24	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>
23	Vinit, K. S. Sujith, C. N. Ramachandran	Spin-spin coupling in nitrogen atom encapsulated C <sub>60</sub> , C <sub>59</sub> N and their respective dimers.	2016, 120, 6990-6997.	<i>J. Phys. Chem. A.</i>
22	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>
21	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>
20	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>
19	K. S. Sujith, C. N. Ramachandran	Carbon dioxide induced bubble formation in a CH <sub>4</sub> -CO <sub>2</sub> -H <sub>2</sub> O ternary system: A molecular simulation study	2016, 18, 3746-3754.	<i>Phys. Chem. Chem. Phys.</i>
18	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>
17	V. Shilpi, S.P. Kaur, C.N. Ramachandran	Revisiting the structural pattern and the stability of (H <sub>2</sub> O) <sub>20</sub> clusters using the dispersion corrected density functional method	2015, 626, 39-42.	<i>Chem. Phys. Lett.</i>
16	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>
15	A. Equbal, S. Srinivasan, C.N. Ramachandran, N. Sathyamurthy	Encapsulation of paramagnetic diatomic molecules B <sub>2</sub> , O <sub>2</sub> and Ge <sub>2</sub> inside C <sub>60</sub>	2014,610-611, 251-255	<i>Chem. Phys. Lett.</i>
14	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>

13	C. N. Ramachandran, B. K. Mishra, A. K. Tiwari	Density functional studies of endosulfan and its interaction with glycine and GABA	<b>2012</b> ,124, 203-207	<i>J. Chem.Sci,</i>
12	C. N. Ramachandran, Eli Ruckenstein	Encapsulation of interstellar abundant H <sub>3</sub> <sup>+</sup> in a C <sub>60</sub> fullerene	<b>2011</b> ,111, 3695-3700.	<i>Int.J.Quant.Chem.</i>
11	C. N. Ramachandran, Eli Ruckenstein	Density functional theoretical studies of the isomers of croconic acid and their dimmers	<b>2011</b> ,973, 28-32	<i>Comp. Theor. Chem.</i>
10	C. N. Ramachandran, Eli Ruckenstein	Water Clustering around CO <sub>2</sub> molecule	<b>2011</b> ,966, 84-90.	<i>Comp. Theor. Chem.,</i>
9	C. N. Ramachandran, D. De Fazio, N. Sathyamurthy, V. Aquilanti	Guest species trapped in carbon nanotubes	<b>2009</b> , 473, 146-150	<i>Chem. Phys. Lett.</i>
8	C. N. Ramachandran, D. De Fazio, S. Cavalli, F. Tarantelli, V. Aquilanti	Revisiting the potential energy surface for the He + H <sub>2</sub> <sup>+</sup> → HeH <sup>+</sup> + H reaction at the full configuration interaction level	<b>2009</b> , 469, 26-30	<i>Chem. Phys. Lett.,</i>
7	C. N. Ramachandran, D. Roy, N. Sathyamurthy	Host-guest interactions in endohedral fullerenes	<b>2008</b> , 461, 87-92.	<i>Chem. Phys. Lett.</i>
6	C. N. Ramachandran, N. Sathyamurthy	A Time-Dependent Density Functional Theoretical Study of BN-Substituted C <sub>60</sub>	<b>2007</b> ,111, 6901-6903	<i>J. Phys. Chem. A.</i>
5	C. N. Ramachandran, N. Sathyamurthy	Introducing a twist in carbon nanotube	<b>2006</b> , 91 1503-1505	<i>Curr. Science.,</i>
4	O. Shameema, C. N. Ramachandran, N. Sathyamurthy	Blue shift in X-H stretching frequency of molecules due to confinement	<b>2006</b> ,110, 2-4	<i>J. Phys. Chem. A,</i>
3	Elango, R. Parthasarathi, V. Subramanian, C. N. Ramachandran, N. Sathyamurthy	Hydrogen peroxide clusters: The role of open book motif in cage and helical structures	<b>2006</b> ,110, 6294-6300	<i>J. Phys. Chem. A,</i>
2	M. Elango, R. Parthasarathi, V. Subramanian, C. N. Ramachandran, N. Sathyamurthy	Atomic and molecular clusters: designer materials for the nanoworld	<b>2005</b> ,71, 405-410	<i>Proc. Indian Natn. Sci. Acad., Part-A</i>
1	C. N. Ramachandran, N. Sathyamurthy	Water clusters in a confined nonpolar environment	<b>2005</b> , 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

### *Teaching (UG/PG Courses)*

<b>Sl. No</b>	<b>Course Code</b>	<b>Course Title</b>	<b>Program</b>	<b>Year/ Semester</b>
43	CYN-001	Physical Chemistry	B. Tech 1 <sup>st</sup> Year, (CH,EPH,MSP)	2022-23/A
42	CY-501	Quantum Chemistry, Symmetry and Group Theory	M.Sc (1 <sup>st</sup> Year)	2022-23/A
41	CYN-302	Group Theory and Spectroscopy	Int. M.Sc- 3 <sup>rd</sup> Year	2021-22/S
40	CYN-001	Physical Chemistry	B. Tech (1 <sup>st</sup> Year) (CH,EPH,MSP)	2021-22/A
39	ICY-303	Introduction of Photochemistry	Int. M.Sc- 3 <sup>rd</sup> Year	2021-22/A
38	CYN-610	Molecular Modeling and Simulations	M.Sc (2 <sup>nd</sup> year) & Pre-Ph.D	2020-21/S
37	ICY-303	Introduction of Photochemistry	Int. M.Sc- 3 <sup>rd</sup> Year	2020-21/S
36	CYN-103	Computer Programming	Int. M.Sc. (1 <sup>st</sup> Year)	2020-21/A
35	CYN-302	Group Theory and Spectroscopy	Int. M.Sc- 3 <sup>rd</sup> Year	2019-20/S
34	CYN-610	Molecular Modeling and Simulations	M.Sc (2 <sup>nd</sup> year) & Pre-Ph.D	2019-20/S
33	CYN-103	Computer Programming	Int. M.Sc. (1 <sup>st</sup> Year)	2019-20/A
32	ICY-303	Introduction of Photochemistry	Int. M.Sc- 3 <sup>rd</sup> Year	2019-20/A
31	CYN-610	Molecular Modeling and Simulations	M.Sc (2 <sup>nd</sup> year) & Pre-Ph.D	2018-19/S



30	CYN-103	Computer Programming	Int. Msc. -(1 <sup>st</sup> year)	2018-19/A
29	CYN-501	Quantum Mechanics, Symmetry and Group Theory	M.Sc-1 <sup>st</sup> year	2018-19/A
28	CYN-741	Chemometrics and Modeling	M.Tech & Pre-Ph.D	2018-19/A
27	CYN-104	Physical Chemistry-I	Int. M.Sc -1 <sup>st</sup> year	2017-18/S
26	CYN-504	Kinetics & Photochemistry	M.Sc-1 <sup>st</sup> year	2016-17/S
25	CYN-782	Chemistry of Industrial Processes	M.Tech & Pre-Ph.D	2017-18/S
24	CYN-103	Computer Programming	Int. Msc. -(1 <sup>st</sup> year)	2017-18/A
23	CYN-501	Quantum Mechanics, Symmetry and Group Theory	M.Sc-1 <sup>st</sup> year/ Int.M.Sc-4 <sup>th</sup> year	2017-18/A
22	CYN-741	Chemometrics and Modeling	M.Tech & Pre-Ph.D	2017-18/A
21	CYN-504	Kinetics and Photochemistry	M.Sc-1 <sup>st</sup> year	2016-17/S
20	CYN-782	Chemistry of Industrial Processes	M.Tech & Pre-Ph.D	2016-17/S
19	CYN-501	Quantum Mechanics, Symmetry and Group Theory	M.Sc-1 <sup>st</sup> year/ Int.M.Sc-4 <sup>th</sup> year	2016-17/A
18	CYN-741	Chemometrics and Modeling	M.Tech & Pre-Ph.D	2016-17/A
17	CYN-504	Kinetics and Photochemistry	M.Sc-I year Int. M.Sc-4 <sup>th</sup> year	2015-16/S
16	CYN-782	Chemistry of Industrial Processes	M.Tech & Pre-Ph.D	2015-16/S
15	CY-001	Physical Chemistry-I	B.Tech	2015-16/A
14	CYN-501	Quantum Mechanics, Symmetry and Group Theory	M.Sc-I year/ Int.M.Sc-4 <sup>th</sup> year	2015-16/A
13	CYN-741	Chemometrics and Modeling	M.Tech & Pre-Ph.D	2015-16/A
12	CY-332	Nuclear and Radio Chemistry	Int. M.Sc-3 <sup>rd</sup> year	2014-15/S
11	CYN-782	Chemistry of Industrial Processes	M.Tech & Pre-Ph.D	2014-15/S
10	CY-001	Physical Chemistry-I	B.Tech	2014-15/A
9	CY-331	Physical Chemistry-II	Int. M.Sc-3 <sup>rd</sup> year	2014-15/A
8	CY-511	Quantum Mechanics, Symmetry and Group Theory	M.Sc-1 <sup>st</sup> Year/ Int. M.Sc 4 <sup>th</sup> year	2014-15/A
7	CY-741	Chemometrics and Modeling	M.Tech & Pre-Ph.D	2014-15/A
6	ICY-03	Introduction to Photochemistry	B. Tech (Inst. Elective)	2013-14/S
5	CY-001	<i>Physical Chemistry-I</i>	<i>B.Tech</i>	<i>2013-14/A</i>

4	CY-511	Quantum Mechanics, Symmetry and Group Theory	M.Sc-1 <sup>st</sup> year/ Int. M.Sc 4 <sup>th</sup> year	2013-14/A
3	CY-637	Advanced Physical Chemistry-I	M.Sc-2 <sup>nd</sup> Year	2013-14/A
2	CY-722	Chemometrics and Modeling	M.Tech & Pre-Ph.D	2012-13/S
1	CY-752	Analysis of Food and Drugs	M.Tech & Pre-Ph.D	2012-13/S

### Research Supervision

<b>Degree</b>	<b>Ph.D Thesis Completed/Submitted</b>	<b>In Progress</b>	<b>Total</b>
<b>Ph.D</b>	5 Completed	5	10
<b>M.Tech</b>	5 completed	0	5
<b>M.Sc</b>	13 completed	2	15

### Details of Thesis Supervised

<b>Degree</b>	<b>Name of the Student</b>	<b>Title of the Thesis</b>	<b>Status</b>
<b>Ph.D</b>	1. Ms. Surinder Pal Kaur	Computational Studies of Selected Gas Hydrates and Hydrate Melts	<b>Completed</b>
	2. Mr. Sujith K. S	Molecular Dynamics Studies of Mixed Gas Hydrate Melts and Aqueous Interfaces	<b>Completed</b>
	3. Ms. Ankita Joshi	Structure and Properties of $\pi$ - $\pi$ Interacting Complexes of Carbon Nanotubes	<b>Completed</b>
	4. Mr. Vinit.	Computational Studies of the Derivatives of Fullerenes and Carbon Nanotubes	<b>Completed</b>
	5. Mr. Mohan Tiwari	Computational Studies of Structure, Stability and Properties of Carbon Intercalated Gold Clusters	<b>Completed</b>
	6. Mr. Angat Dhiman	Charge Transport Properties of Selected Molecules Sandwiched Between Various Electrodes	<i>In Progress</i>
	7. Mr. Peaush Gangwar	Modeling of Catalytic Systems for Mitigation of Environmentally Hazardous Gases	<i>In Progress</i>
	8. Mr. Paras	Computational Designing of Different Fluorescent Molecules	<i>In Progress</i>
	9. Mr. Shivam Rawat	Modeling of CO <sub>2</sub> absorption using Aqueous Amines	<i>In Progress</i>
	10. Mr. Aashu	Molecular dynamics simulations studies of clustering of gas molecules in water	<i>In Progress</i>

	11. Sanjay Sharma	<i>Designing of Covalent Organic Frameworks</i>	<i>In Progress</i>
	12. Vivek	<i>Two and Three Photon Absorption</i>	<i>In Progress</i>
<b>M. Tech</b>	1. Mr. V. Shilpi	<i>Structural Pattern and the Stability of Water Clusters in Gas Hydrates</i>	<b>Completed</b>
	2. Ms. Bhawana Singh Tomar	<i>Promoters and Inhibitors of Gas Hydrates</i>	<b>Completed</b>
	3. Ms. Suman Lata	<i>Clustering of Some Atmospherically Important Molecules: A Computational Study</i>	<b>Completed</b>
	4. Mr. Rajdeep Shehrawat	<i>Interaction of Carbon Nanotube with Tau Protein: A Molecular Dynamics Simulation Based Study</i>	<b>Completed</b>
	5. Mr. Rajat Pundhir	<i>Effect of roughness of interface on the dissolution of gas molecules: The case of CO<sub>2</sub></i>	<b>Completed</b>
<b>M. Sc</b>	1. Ms. Sakshi Ganotra	<i>Interaction of Endosulfan with Flat and Curved Carbon Surfaces</i>	<b>Completed</b>
	2. Ms. Manisha Prakashni	<i>Structure and Optical Properties of Oxadiazole and its Derivatives: A Computational Study</i>	<b>Completed</b>
	3. Mr. Mohit Rohilla	<i>A Computational Study of Interaction Between Natural Collagen of Type-I and Carbon Nanotube</i>	<b>Completed</b>
	4. Mr. Laukesh Kr. Sharma	<i>A Preliminary Theoretical Study of Pd<sub>n</sub>C<sub>m</sub> (n,m = 1-5) Clusters</i>	<b>Completed</b>
	5. Mr. Vishal Kumar Yadav	<i>Density functional studies of the dissociation of selected compounds</i>	<b>Completed</b>
	6. Mr. Anshul Aggarwal	<i>Computational Studies of Covalently and Non-covalently Linked Stacked Porphyrin Dimers</i>	<b>Completed</b>
	7. Mr. Ankita Narwal	<i>Structure and Stability of Carbon Supported Platinum Clusters: A Computational Study</i>	<b>Completed</b>
	8. Mr. Vishnav	<i>Generation Mechanism of Selected Amino Acids in the Interstellar Medium: A Theoretical Study</i>	<b>Completed</b>
	9. Ayishwarya Dutta	<i>Computational studies of selected organic fluorophores based on coumarin</i>	<b>Completed</b>
	10. Sandeep Singh	<i>Adsorption of H<sub>2</sub> and CO<sub>2</sub> over small clusters of TiO<sub>2</sub>: A density functional theoretical study</i>	<b>Completed</b>
	11. Sheetal Kalra	<i>Computational studies of porphyrin fullerene host-guest complexes</i>	<b>Completed</b>
	12. Pradyumn Kasaundan	<i>Modeling of phenyl substituted norbornadiene and quadricyclane and their respective dimers</i>	<b>Completed</b>
	13. Chinky	<i>Effect of substituents and hydrogen bonding on the energy storage capacity of Norbornadiene-Quadricyclane system: A computational study</i>	<b>Completed</b>
	14. Divyanshu Joshi	<i>Effect of nonpolar solvents on frontier molecular orbitals</i>	<b>In Progress</b>
	15. Arju	<i>Chiroptical properties of selected compounds</i>	<b>In Progress</b>

### Seminars/conferences

No	Name of the conference	Institute	Participation/presentation	Date
19.	Theoretical Chemistry and Biology Symposium(TCB)	IISER Mohali, NIPER Mohali and IIT Ropar	Presentation	15.10.2022
18.	Faculty Development Program	UGC-Human Resource Development Centre, Panjab University	Resource Person	21 Sep 2022 - 21 Sep 2022
17.	17th Theoretical Chemistry Symposium (TCS-2021)	IISER Kolkota, IACS Kolkota, University of Kalyani, SNBNCBS Kolkota	Chairperson	December 11-14, 2020
16.	Online Refresher Course in Chemical Science	UGC-Human Resource Development Centre, Kannur University, Kerala	Presentation	21.08.2020
15.	Meet IIT Roorkee Rising Stars	Department of Chemistry, IIT Roorkee	Presentation	02.08. 2020
14.	Webinar Series on Computational Chemistry	Mar Ivanios College, Trivandrum, Kerala	Presentation	April 2020- June 2020
13.	Advanced Simulation Methods	IIT Delhi	Presentation	8-10 March, 2019
12.	Theoretical Chemistry Symposium (TCS-2018)	BITS Pilani	Presentation	13-16 February, 2019
11.	International Conference on Physics and Chemistry of Materials (ICCPM-2019)	St. Thomas College, Thrissur, Kerala	Presentation	19-21 December, 2018
10.	National Seminar on Material Science and Technology for Sustainable Future	Malabar Christian College, Calicut, Kerala	Presentation	18 December, 2018
9.	Institute Visit	IIT Ropar	Presentation	10 July, 2018
8.	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 Kolkota, SINP Kolkota, IACS Kolkota	Presentation	14-18 February, 2018
6.	8 <sup>th</sup> Asia Pacific Conference on Theoretical and Computational Chemistry	Indian Institute of Technology Bombay	Presentation	14-17 December, 2017
5.	Workshop on Computational Chemistry	Institute for Integrated Programmes and Research in Basic Sciences, M.G. University, Kottayam, Kerala	Lecture	22 June, 2017
4.	North West Meeting on Structure, Spectroscopy and Dynamics	BITS Pilani	Presentation	20-22 February, 2017

3.	Theoretical Chemistry Symposium	Hyderabad Central University, IICT Hyderabad, IIT Hyderabad	Participation	13-17 December, 2016
2.	JSPS-DST Asian Academic Seminar	IACS Kolkota & IISER Kolkota	Participation	6-10 March, 2015
1.	Theoretical Chemistry Symposium	NCL Pune & IISER Pune	Participation	18-21 December, 2014

### 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

### Responsibilities at Institute and Department Levels

No.	Administrative Responsibilities	Year
15.	Associate Dean of Academic Affairs (Curriculum)	2020-
14.	Member, Advisory Committee, Institute Computer Centre	2020-
13.	Member, Institute Research Committee, IIT Roorkee	2014 -2018
12.	Member, Advisory Board, Continuing Education Centre, IIT Roorkee	2015-2018
11.	Deputy Chief Advisor, Cinema Club, IIT Roorkee	2014-2017
10.	Dept. Representative, ERP, IIT Roorkee	2015-
9.	Member, Review Committee for Ph.D Admission Process	2018
8.	Member, Review Committee for External Ph.D Supervision	2018
7.	Convener, Department Faculty Search Committee, Chemistry, IITR	2014-2016
6.	In Charge, Department Research Committee, Chemistry, IITR	2015-2018
5.	Member, Department Research Committee, Chemistry, IITR	2014-2022
4.	In Charge, Chemistry Association, IITR	2014-2018
3.	Member, Department Administrative Committee, Chemistry, IITR	2016-2018
2.	Member, Student Research Committees, Chemistry and Physics, IITR	2013-
1.	Joint Secretary, International Conference on Advanced Materials for Energy, Environment and Health (ICAM-2016)	2016

### Conferences Organized/Organizing

Convener, 3<sup>rd</sup> 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

**Guest Editor:** Topical issue on 'Atoms and Molecules in a confined environment', European Physical Journal D (2021)

**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/Memberships

**1. Outstanding Teacher Award, IIT Roorkee (2019)**

2. Life Member, CRSI

3. Biography selected in the 2010 edition of Marquis Who's who in the world.

4. Fellowship from the Research Foundation, State University of New York

5. Fellowship from the Italian Ministry of University and Research

6. Cleared National Eligibility Test with Research Fellowships

7. Sree Guruvayurappan Scholarship for the Best Student in B.Sc Chemistry, Sree Krishna College Guruvayur, Kerala