

# Jayasree Elambalassery

Professor  
Dept. of Applied Chemistry  
CUSAT  
Email: [jelambal@cusat.ac.in](mailto:jelambal@cusat.ac.in),  
[jelambal@gmail.com](mailto:jelambal@gmail.com)  
Phone: 97467 90202

Elambalassery House  
P.O.Meladoor  
Thrissur Dist  
Kerala-680 741

## SUMMARY

- ⇒ Three years and nine of months of post-doctoral research
- ⇒ Eleven years of teaching experience
- ⇒ Proven track record in computational modeling and design
- ⇒ Hands on experience on many computational packages and operating system environments
- ⇒ Well-organized and strong problem solving potential
- ⇒ Experience on mentoring undergraduates, post graduates, M.Phil. and Ph.D. scholars

## POST DOC WORK EXPERIENCE

### Research:

**2004-2006: Post doctoral research fellow, *University of California, Berkeley***

(Supervisor: Prof Andrew Streitwieser): Carried out theoretical investigations on: substituent effects on the ionic and ion-pair  $S_N2$  reactions of allyl halides; effects of solvation on the energy barrier and reaction mechanism of ion pair  $S_N2$  reactions; the aggregation and reactivity of metal enolates; solvent effects on keto-enol tautomerism of acetyl acetone and equivalent structures; effects of various effective core potentials on cesium compounds and its application for the calculation of cesium ion pair acidities.

**2006-2008: Post doctoral research fellow, *Trinity University, San Antonio, Texas***

(Supervisor: Prof Steven M. Bachrach): Applied computational chemistry packages to investigate: Solvation effects on nucleophilic exchange reactions; Influence of hydrogen bonding /non-covalent interactions on the reactivity and properties of cystines and related biomolecules.

**2011-2012: Independent research work along with supervision of PG research projects (Completed two PG research projects).**

### Teaching:

1998: Guest Lecturer in Carmel College, Mala (affiliated to University of Calicut, Kerala, India)

Jan – June 2007: Part-time Faculty in Trinity University, San Antonio, Texas.

Sept-Dec 2010: Assistant Professor at MES College of engineering, Kuttippuram

Jan 2011-Aug 2012: Assistant Professor at Mercy College, Palakkad.

Sept 2012 – June 2022 : Assistant Professor at the Department of Chemistry, University of Kerala.

From June 2022 onwards : Professor at Department of Applied Chemistry, CUSAT

### HONOURS and AWARDS

- Certificate of appreciation from the Vice Chancellor, Univ. of Kerala for providing significant contribution in the quality enhancement of University of Kerala during the year 2014-2018. (2018)
- Junior Research Fellow of the Council of Scientific and Industrial Research, India (1999-2001)
- Senior Research Fellow of the Council of Scientific and Industrial Research, India (2001-2004)
- Eligibility for Lectureship, University Grants Commission, India (1998)
- Kanakam Thamburan Memorial Award for the best student in theoretical Chemistry, University of Calicut, India(1998)
- Second Rank in the Master of Science examination, University of Calicut, India(1998)
- Fourth Rank in the Bachelor of Science examination, University of Calicut, India(1996)

### PUBLICATIONS

1. "Cationic *Closo* Carboranes- Promising Weakly Coordinating Ions".Jemmis, E. D.; Ramalingam, M.; Jayasree, E.G.; *J. Comput. Chem.*; 2001; 22; 1542-1551.
2. "The Relation between Polyhedral Borane Sandwiches and Endohedral Complexes; the Electronic Structure and Stability of  $X@YmBnHn+mq$  ( $X=He,Ne,Li,Be$ ;  $Y=B,C,Si$ ;  $m=0-3$ ;  $n=12-9$ ;  $q=-2$  to  $+2$ ); ( $C2B4H6$ ) $2Xq$ ( $X=Li,Al,Si$ ;  $q=-3,-1,0$ ) and  $X2@B17H17q$  ( $X=He,Li$ ;  $q=-2,0$ )." Jemmis, E. D.; Jayasree, E. G.; *Collect. Czech. Chem. Commun.*; 2002; 67, 965-990.
- 3."Ab initio Molecular Orbital Studies on the Structural Isomers of  $C3Si2H4$ " Jemmis, E. D.; Saradha, R.; Saieswari, A.; Jayasree, E. G. *Ind.J. Chem.A* . 2003, 42A, 2382-2391.
4. "Analogies between Boron and Carbon." Jemmis, E. D.; Jayasree, E.G. *Acc.Chem. Res.* 2003, 36, 816-824.\*
5. "The Rearrangement of Dicarboranyl Methyl Cation: A Possible Synthetic Strategy towards Cationic *closo*-Tricarbaboranes". Jemmis, E. D.; Jayasree, E. G.*Inorg. Chem.* 2003, 42, 7725-7727.
6. "Does a sterically bulky group occupy the equatorial site in trigonal bipyramidal phosphorous?". Kommana, P.; Satish Kumar, N.; Vittal, J. J.; Jayasree, E. G.; Jemmis,E.D.; Kumara Swamy, K. C. *Org. Letters*. 2004, 6, 145-148.
7. "Hypercarbons in polyhedral structures." Jemmis, E. D.; Jayasree, E. G.; Parameswaran,P. *Chem. Soc. Rev.* 2006, 35, 157-168. \*\*
8. "A Theoretical study of substituent effects on allylic ion and ion pair SN2 Reactions" Streitwieser, A.; Jayasree, E. G.; S.S.-H. Leung; G. S.-C.Choy. *J. Org. Chem.* 2005, 70, 8486-8491.
9. "Evaluation of two computational models based on different effective core potentials for use in organocesium chemistry". Streitwieser, A.; Liang, J. CY.; Jayasree, E. G.; Hasanayn, F. *J. Chem. Theory. Comput.* 2007, 3, 127-131.
10. "Theoretical study of the effect of coordinating solvent on ion-pair SN2 reactions: The role of unsymmetrical transition structures" Streitwieser, A.; Jayasree, E. G. *J. Org. Chem.* 2007, 72, 1785-1798.
11. "A Theoretical Study of SN2 reactions of allylic halides: ' the Role of Ion Pairs" Streitwieser, A.; Jayasree, E. G.; Hasanayn, F.; Leung, S.S.H, *J. Org. Chem.* 2008, 73, 9426-9434.

12. "Cationic Closo-carboranes 2. Do computed  $^{11}\text{B}$  and  $^{13}\text{C}$  NMR chemical shifts support their experimental availability?" Hnyk, D; Jayasree, E. G. *J. Comput. Chem.* 2013, 34(8), 656-661.
13. "A Computational Study on the Enolization of Acetone – Reaction Mechanism and Substituent Effects." Jayasree E. G.; Dhanya M. *Scientia* 2013. (ISSN: 0976-8289)
14. "A computational study on the reaction mechanism and energetics of Markovnikov and anti-Markovnikov addition in alkyne hydrothiolation reactions" Jayasree E. G.; Reshma, S. *Comput. Theor. Chem.*, 2016, 1098, 13-21. <http://dx.doi.org/10.1016/j.comptc.2016.10.012>.
15. "Density functional evaluation and a feasibility study of intramolecular thione-thiol tautomerization" Jayasree E. G.; Soorya S. *Int. J. Quantum. Chem.* 2017, 117 (20), e25427-e25438.. <https://doi.org/10.1002/qua.25427>
16. "Qualitative and quantitative study on C-C rotation during tautomerization of thione, selenone, and tellurone" Jayasree E. G.; Soorya S. *J. Stru. Chem. (Springer)* 2018, 59 (7), 1534-1543.
17. "A computational study on the reaction mechanism and energetics of alkyne hydroselenation reactions" Jayasree E. G.; Mohanan A.; Reshma S. *Comput. Theor. Chem.*, 2017, 1118, 166-174.
18. Jayasree, E.G.; Sreedevi, S. "Computational study on ionic and ion pair methylation reactions of enethiolates and their lithium salts." *Theoretical Chemistry Accounts* 137, (2018), 160-173.
19. Surya Philip; Jayasree E. G.; Mohanan, K. "Antidiabetic, antioxidant, DFT and molecular docking studies of a triazene derivative and its transition metal complexes" *Research on Chemical Intermediates*, July 2019. [10.1007/s11164-019-03936-8](https://doi.org/10.1007/s11164-019-03936-8) 46, 75-99, 2020
20. Balachandran, A. L.; Athira, C. S.; Deepthi, A.; Jayasree E. G. "A convenient synthesis of 2,5-diaroyl-4-hydroxy cyclopent-2-enones incorporating aromatic and heteroaromatic moieties" *Synthetic Communications* 2019, <https://doi.org/10.1080/00397911.2019.1670851> , 49(24), 3401-3411.
21. Jayasree, E. G.; Sreedevi, S. "A DFT Study on Protic Solvent Assisted Tautomerization of Heterocyclic Thiocarbonyls" *Chemical Physics*, 2020, 530 <https://doi.org/10.1016/j.chemphys.2019.110650>
22. Jayasree, E. G.; Mohanan, A "Computational study on atom-economic alkyne hydrotelluration reaction using benchmarked ECP for Te" *J. Mol. Graph. Model.* 2020, 100, 107659. <https://doi.org/10.1016/j.jmgm.2020.107659>
23. Jayasree, E. G.; Sukumar, C. "A DFT study on the cleavage of dichalcogenide bridges in cystines and selenocystines: Effect of hydrogen bonding" *Inorg. Chim. Acta*, 2020, 512, 119897, <https://doi.org/10.1016/j.ica.2020.119897>
24. Jayasree E. G.; Sukumar, C; Asha, S. "A theoretical insight into the reducing properties of bicyclic dithia hydrocarbons and hetero-bicyclic dithiopyrrolone compounds with rotation-restricted planar disulfide linkage" *Structural Chemistry*, 2021, 32, 107-113 DOI: 10.1007/s11224-020-01613-w
25. Balachandran, A.L.; Jayasree E. G.; Deepthi, A., An insight into the dual fluorescence of 3,6-dihydroxybenzene-1,2,4,5-tetracarboxylic acid tetraethyl ester – an experimental and theoretical study *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* 2021
26. Jayasree, E. G.; Reshma, S.; Mohanan, A. "Computationally Unravelling the Mechanism and Selectivity of Five and Six membered N-Heterocyclic Carbene- Catalyzed Alkyne Hydrochalcogenation" *Int. J. Quantum Chem.*, Accepted 2021 <https://doi.org/10.1002/qua.26652>

27. Jayasree, E. G.; Sukumar, C. "Integrating redox-response in crown ethers by disulfide incorporation: A computational approach" *Structural Chemistry*, Accepted 2021. [10.1007/s11224-021-01761-7](https://doi.org/10.1007/s11224-021-01761-7)

28. Remiya, J. P.; Sikha, T. S.; Shyni, B.; Anitha, L.; Nair Lakshmi, C. S.; Jayasree, E. G. "Synthesis, spectral characterization and biological evaluations with DFT analysis on molecular geometry and NLO of 1,4,7,10-tetraazacyclotetradecane-11,14-dione" *J. Ind. Chem. Soc.* 2021, 98, 100132 <https://doi.org/10.1016/j.jics.2021.100132>.

29. Surya Philip; Jayasree E. G., Mohanan, K. Antiproliferative studies of transition metal chelates of a pyrazolone based hydrazone derivative *Journal of biomolecular structure and Dynamics*, 2022, <https://doi.org/10.1080/07391102.2021.2024257> (IF:3.392)

\* Report: *Chemical & Engineering News* has a report on our 2003 Acc. Chem. Res. Paper by Stephen K. Ritter (2004, 82, 28-32)

\*\* CSR issue has its cover picture on the related article (Issue2, 2006) and has been selected as best cover picture for beautiful science in 2006.

### As resource person:

1. IISER, Bhopal April 2010- "Influence of Weak Interactions: A Computational Study on Nucleophilic Exchange Reactions in Dichalcogenides"
2. MHRD sponsored "Current Trends in Organometallic Chemistry", NIT, Calicut, 05-07-11 : "Computational Organometallics: An over view of theoretical methods" 06-07-11: "Computational Organometallics: Practical Approaches"
3. A talk as a part of Lecture Series conducted in association with IYC 2011 at Mercy College, Palakkad- "Perspectives on Computational Chemistry".
4. Talk on "Perspectives on Quantum Chemistry: A cake-walk into the virtual reality of the chemical world." In "SPECTRUM 2013" seminar series at SN College, Chempazhanthy.
5. KSCSTE and DST sponsored two day International conference "New horizons in Chemistry" at St. Joseph's College, Irinjalakuda, Sept 2013- "A DFT approach on the influence of non-covalent interactions in redox and nucleophilic exchange reactivity of cystines and selenocystines".
6. Delivered lectures (15 hrs) on "Molecular modelling" to M. Tech and Ph.D. students as part of their course completion at IIST, Valiamala, Thiruvananthapuram (1-11 Oct 2013).
7. Delivered a lecture on "Molecular modelling" to M.Phil-CADD and M.Sc. students at Department of Computational Biology and Bioinformatics, University of Kerala on 6-11-2013.
8. Delivered a lecture on "Molecular Modelling" at SN college, Chengannur on 14-11-2013
9. Delivered lectures on various topics of Quantum Mechanics as part of the UGC Remedial Coaching program at Kannur University, Payyanur Campus on 7<sup>th</sup>, 8<sup>th</sup>, 14<sup>th</sup> and 15<sup>th</sup> December, 2013.
10. Delivered lectures on various topics of Quantum Mechanics in Science Academies' Lecture Workshop on "Recent Developments in Physical Chemistry" sponsored by National Academy of Sciences, Allahabad, Indian Academy of Sciences, Bangalore and Indian National Science Academy, New Delhi on January 31<sup>st</sup> and February 1<sup>st</sup> 2014 held at Research & PG Department, St. Joseph's College, Irinjalakuda.
11. Delivered a lecture on "Orbital Interactions- Deciphering the Chemical Puzzles" in One day National Seminar on "Recent Trends in Chemistry" held at Carmel College, Mala on 26<sup>th</sup> February 2014.
12. Delivered lectures on various topics of "Chemical Bonding" and "Group Theory" as part of the UGC remedial coaching program at School of Chemical Sciences, M. G. University, Kottayam on 24<sup>th</sup> May, 2014.
13. Delivered 10 hour lecture series on "molecular modelling" for a course on Mathematical modelling and simulation to M.Tech students at IIST, Valiamala from 17<sup>th</sup> – 19<sup>th</sup> November, 2014.

14. Delivered a lecture on 'Modeling and Simulation' at the refresher course in nanoscience organized at the Academic Staff College, University of Kerala on 27/11/2014.
15. Delivered lectures on "An Introduction to Computational Chemistry" and "Modern Approach to Computational Chemistry" in two day national seminar on "New Frontiers in Chemistry" on 2-3 March, 2015 held at University College, Thiruvananthapuram.
16. Delivered lecture on "Redox properties of cystines and sulphur containing cages – A DFT study" in UGC sponsored two day National Conference on Smart Materials(NCSM-2015) organized by Dept of Chemistry, Univ. of Calicut on 24<sup>th</sup> March, 2015.
17. Delivered lectures on various topics of "Chemical Bonding" and "Group Theory" at School of Chemical Sciences, Kannur University, on 23<sup>rd</sup>, 25<sup>th</sup> and 26<sup>th</sup> March, 2015 under Visiting Faculty programme.
18. Delivered lectures on 'Approximation methods' at a National Workshop on Quantum Mechanics 2015 conducted by Srinivasa Ramanujan Institute for Basic Sciences (SRIBS) of KSCSTE at Kottayam on 20-21 June, 2015.
19. Delivered a lecture on 'Potential energy surface' and provided hands-on training on Gamess software in UGC sponsored National Seminar on 'Machine Learning Approaches a New Trend in Quantum Mechanics' organized by SN College, Chengannur held on Aug 04 -06 , 2015.
20. Delivered lectures on 'Group Theory – Chemical Applications' at a National Workshop on Group Theory conducted by Srinivasa Ramanujan Institute for Basic Sciences (SRIBS) of KSCSTE at Kottayam on 30 October-1 November, 2015.
21. Delivered a lecture on 'From molecules to solids: A computational chemist's view' at the refresher course in nanoscience organized at the Academic Staff College, University of Kerala to be conducted in Nov-Dec, 2015.
22. Delivered a lecture on 'Spectral property prediction by computational methods' at a National workshop on Recent Advances in Phytochemical Profiling of Medicinal Plants at Dept of Botany, University of Kerala on Jan 7<sup>th</sup> 2016.
23. Talk on 'Computational Chemistry and Gaussian Program Package' in the seminar organized by Dept.of Chemistry, Mercy College, Palakkad on 22<sup>nd</sup> January 2016.
24. Talk on 'Approximation Methods in Quantum Chemistry' in the Govt. of Kerala sponsored 2-day national seminar on Transcending Areas in Chemistry organized by Dept. of Analytical Chemistry, Govt. Arts College, Thiruvananthapuram on 14<sup>th</sup> March 2016.
25. Talk on 'MOT perspective on the approximate solutions of molecular Schrodinger equation' in UGC sponsored National Seminar on 'Computational Chemistry' at MG College, Thiruvananthapuram held on 8-9 June 2016.
26. Attended and chaired a session in the international conference 'Computational Modeling of Molecules and Materials –CM<sub>3</sub>-2016' held at the Riverview retreat at Corbett National Park, Nainital during October 20-22, 2016 organized by IIT, Indore.
27. Talk on "Introduction to Quantum Mechanics and Beyond" in the Seminar series conducted at S.N. College, Varkala on 23<sup>rd</sup> November, 2016.
28. Delivered a lecture on 'Hartree Fock Theory' at a workshop on Computational Chemistry and Applications organized by Srinivasa Ramanujan Institute for Basic Sciences(SRIBS) at Pampady, Kottayam on 30 Dec-1 Jan 2017
29. Delivered a lecture on 'Computational Chemistry' at a Lecture workshop organized at Bishop Moore College, Mavelikkara as part of K.C. Mathew endowment lecture on 13<sup>th</sup> March, 2017.
30. Delivered a lecture on "Iron complexes: Promising regiospecific catalysts for hydrochalcogenation" at UGC sponsored National Seminar on 'Frontiers in Chemistry 2017' organized by Department of Chemistry, University of Calicut on 28-30 March, 2017.
31. Delivered a lecture on "From molecules to solids: A computational Chemist's view" at MRSI sponsored National Seminar on Advanced Functional Materials(NSAFM 2017) at Mar Ivanios College, Thiruvananthapuram on 12-14 December, 2017.
32. On 'Computational Chemistry' at the National Seminar titled 'Dr Siby Joseph Memorial Lecture Series III' sponsored by Dr. Siby Joseph Memorial Charitable Trust and organized by PG and research department of Chemistry, St. Joseph's College, Moolamattom on 16-17 February, 2018.
33. On 'Electronic Structure of Solids – an unmistakable link from atoms and molecules' at the National Seminar on 'Frontline approaches in material science and computational Chemistry'

held at Research & PG Dept. of Chemistry, SN College for Women, Kollam from 14 to 16 March, 2018 sponsored by KSCSTE and ANERT.

34. On 'Approximation Methods' at the National seminar on 'Theoretical Arsenals of Modern Chemistry' organized by PG Department of Polymer Chemistry, Govt. College, Attingal during Oct 23-25, 2018.

35. On 'MOT perspective on the approximate solutions of molecular Schrodinger equation' at the National Seminar on 'Recent Trends in Chemistry, RTC-2018' organized by PG Department of Chemistry, Govt College, Kattappana, on 13-14<sup>th</sup> Nov, 2018.

36. On 'HF and post-HF methods' at the National Seminar on 'Theoretical and Computational Chemistry' held at Govt. College for Women, Thiruvananthapuram during Nov 29-Dec 1, 2018.

37. On 'Fundamental aspects of Computational Quantum Chemistry' at the KSCSTE sponsored National Seminar on Current Trends in Organic and Computational Chemistry, CTROC 2019 organized by Dept of Chemistry, Morning Star Home Science College, Angamaly held during 14-15 Feb, 2019.

38. On 'Enethiolization Reactions and Capricious Structures of Enethiolates' at the National conference on Frontiers in Chemical Sciences-2019 organized by Dept. of Chemistry, University of Calicut during 19-21 March, 2019.

39. On 'Hartree-Fock and post Hartree-Fock methods' at the 3 day state level workshop on Molecular modeling using Gamess and Gaussian organized by PG and Research Dept of Chemistry, Govt. College, Madappally during 19-21 March 2019.

40. Delivered lectures on various topics of 'Computational Chemistry' in a Faculty Development Programme organized by the Department of Chemistry, Amrita School of Arts and Sciences, Amrita Vishva Vidyapeetham, Amrityapuri on June 21 and 22, 2019

41. Delivered a lecture on 'HF and Post HF methods' in one day National Seminar in Computational Chemistry organized by the Dept. of Chemistry, Catholicate College, Pathanamthitta on Jan 10, 2020.

42. Delivered a lecture on 'Basis sets: Instruments for adequate predictions' in the National Workshop (online) on Computational Chemistry organized by SRIBS, KSCSTE in collaboration with IIITM-K on 7<sup>th</sup> Oct, 2020.

43. Delivered a lecture on 'Basis sets' in the Refresher course conducted by UGC-HRDC, Univ. of Kerala on Material Science on 19<sup>th</sup> Oct, 2020.

44. Served as a resource person for the webinar on Computational Chemistry organized by Academy of Chemistry Teachers (ACT) held on 21-11-2020.

45. Invited Lecture in National workshop (online) Computational Modeling in Chemistry, Biology and Materials on "Computations in Reaction Mechanism Studies" organized by CUSAT, sponsored by DST-SERB during 22-28 Nov 2021.

46. Resource person for the scientific talk on Computational Chemistry conducted by Dept of Chemistry, BCM College, Kottayam on 14<sup>th</sup> Jan 2022.

47. Invited Lecture on "Molecular Modeling: Applications in Research and Education" in a National Seminar organized by Dept of Chemistry, VV Vaniaperumal College, Virudhunagar, TN on 16-02-2022

## **Other activities**

1. Member of the editorial board, *Scientia* in 2011. (ISSN No: 0976-8289)

2. Examiner in setting the M.Sc. question papers of various universities(Kannur University) :
3. Member of Programme Advisory Committee Meeting as an examiner in setting the Quantum Chemistry-I and Quantum Chemistry-II M.Sc. question papers of Pondicherry Central University, November 2013.
4. Subject expert in various interview boards
5. Chairman, BQPS of various universities
6. Member, Board of Studies, St. Joseph's College, Irinjalakuda, 2016-till now.; Fatima Mata National College, Kollam from 2022 onwards.
7. Member, Judging Panel, Regional level National Children's Science Congress, 2018 conducted during 4-5 Oct, 2018 at KV Pangode.

### **University Level activities @ University of Kerala**

Head, Dept. of Chemistry, Univ. of Kerala 2021-22

Member, Faculty of Science, 2020-22

Member, Academic Council, 2021-22

Member- NAAC criteria team-2015

Member – Graduate Attribute Committee, IQAC, 2015.

Member –ASAP Committee of IQAC, 2016.

Member- Chancellor Award Committee, 2016-22

Member, PG Board of Studies, Univ. of Kerala, 2018-22

Member, Chancellor's Quarterly Performance Report Committee, 2019-22

Member, SubCommittee for NAAC uploading and documentation, 2022

Member, NAAC committee for 'Centres', 2019

Member, NIRF Committee, 2022

Member, Internal Complaints Committee (ICC), 2022

Department Level apart from normal routine classes, course charges and mentoring:

1. Compiling AQAR reports 2014-2016
2. Compiling Annual reports 2014-16
3. Compiling trimonthly reports 2015-22
4. Admission charge , 2015-22

### **Extension:**

1. Delivered a talk to 7<sup>th</sup> Std School students on 'Chodyangaliloode ariyam, valaram' as part of Department Science day celebrations on 1<sup>st</sup> March, 2017.
2. Published an invited popular article on 'Aavarthanappattikayude charithravazhikal' in Sasthrakeralam, Page no: 13-16, June, 2019
3. Conducted 'Periodix'-National level quiz competition on periodic table for B.Sc. students on 01-03-2019
4. Taken a class on "Quantum mechanics" in the CSIR orientation course conducted by Dept. of Chemistry, University of Kerala on 24-08-2019
5. Delivered a 'keynote address' to 'panchayat level Sasthrolsavam' conducted by 'Sasthra Sahitya Parishat' at Govt. U.P.School, Kariavattom on 28-09-2019.
6. Delivered a talk on "From hard molecular models to electronic visualizations- A journey from knowledge to applications" in a School level webinar on 'COVID-19 : The viral challenge and the scientific defense' organized by Dept. of Chem, Univ. of Kerala on 13<sup>th</sup> June, 2020.

## EDUCATION

\* **Ph.D. in Computational Chemistry** from Central University, Hyderabad, India under the supervision of **Prof Eluvathingal D. Jemmis** (2004). Title of the Thesis: **“Theoretical Studies on Tricarba-substitution, Encapsulation and Condensation in Polyhedral Boranes.”**

### Sponsored Projects :

1. Centre for modelling simulation and design, CMSD-Hyderabad approved the project “Effect of various non bonding interactions on the PKa values of various substituted and unsubstituted cysteines and homocysteines” and provided 15000 CPU hours of computing time with parallel architecture of 8 processors, 5GB memory and 50GB scratch space.
2. SERB/Fast-track (DST) project (Designing Inexpensive Transition Metal Catalysts for C-Z (Z = S, Se, Te) bond formation using atom economy addition reactions: A computational investigation); Sanctioned amount 24,43,000/-.

### Orientation/Refresher Program

1. **Attended 139<sup>th</sup> Orientation program conducted** by ASC, University of Kerala held during 14-10-2014 to 10-11-2014.
2. **Attended Refereshor program conduced by** , University of Kerala held during-31st refresher course in material science (29/11/2016-19/12/2016)
3. **Attended Refereshor program on ‘Materials science conducted by HRDC**, University of Kerala held during-33<sup>rd</sup> refresher course in material science (21/11/2019-04/12/2019)
4. **Attended Refresher Program on LMS**
5. **Attended ARPIT refresher program**



## Research Guidance

### Ph.D. Completed

SI No.	Title	Name of co-guides (if any)	Name of student	University	Year
1.	Theoretical Study of Thione-Thiol Tautomerization and Reactivity of Enethiolates towards Methylation and Aggregation	Nil	Soorya S.	Univ. of Kerala	2020
2.	Synthesis, Characterization and Biological Studies of Some Transition Metal Complexes	Prof. K. Mohanan	Preethy Soosan Thomas	Univ. of Kerala	2019
3.	Synthesis, Characterization and Biological Studies of Metal Based Bioactive Materials	Prof. K. Mohanan	Surya Philip	Univ. of Kerala	2021
4.	Computational Studies on the Reducing Properties of Cystine and Disulfide Incorporated Selected Cyclic and Polyhedral Compounds	Nil	Chinthu Sukumar	Univ. of Kerala	2022

<b>Ph D – Thesis submitted</b>					
SI No.	Title	Name of co-guides (if any)	Name of student	University	Year
1.	Computational Study on the Mechanistic and Energetic Aspects of Alkyne Hydrochalcogenation: Uncatalyzed, and Iron Complex and NHC Catalyzed Pathways	Nil	Reshma S.	Univ. of Kerala	2021
2.	Computational Study on the Mechanistic and Energetic Aspects of Alkyne Hydrochalcogenation: Uncatalyzed, and Cobalt Bidentate Complex and Six- membered NHC Catalyzed Pathways	Nil	Aswathy Mohanan	Univ. of Kerala	2021

1. M.Phil/PG dissertation

<b>M.Phil./P.G. Dissertation</b>					
<b>SI No.</b>	<b>Title</b>	<b>Name of co-guides (if any)</b>	<b>Name of student</b>	<b>University</b>	<b>Year</b>
<b>M.Phil</b>					
1.	A DFT analysis of the stability and reducing properties of thiacycles	-	Asha S.	Univ. of Kerala	2015
2.	A DFT study of reaction mechanisms of disulfide addition to alkynes	-	Varsha Lisa John	Univ. of Kerala	2016
3.	A DFT study on the catalytic efficiency of N-substituted 2,3-Dihydrothiazol-2-ylidenes in alkyne hydrochalcogenation reactions	-	Sumi R.	Univ. of Kerala	2017
4.	A DFT study on the performance of abnormal N-Heterocyclic Carbenes in catalyzing alkyne hydrochalcogenation	-	Anija Rajendran	''	2019
5.	A computational study on the P-heterocyclic carbenes catalyzed C-S bond formations	-	Neethu Mariyam Joseph	''	2020
6.	Probing the redox response and heteroditopic receptor properties of disulfide incorporated crown ether embedded 5-bromo-1,2,3-triazole: A computational study	-	Libin Thomas	''	2021