CURRICULUM VITAE

Current Position: Women Scientist (WISE PDF)

Personal Details:

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W/O. D.Thirumeignanam,
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Current area of Research: **Molecular Quantum Mechanics-Drug design**

Current Position Since October 2024: Women Scientist (WISE-PDF)
Department of Physics
Manonmaniam Sundaranar University,
Tirunelveli

Mentor: Prof.B. Sundarakannan

Details of Ph.D. Degree:

Date of submission of Ph.D. Thesis : 12.08.2011
Month and year of Ph.D. Degree awarded : 09.01.2012
Subject and Title of the Thesis : **Interaction Studies of Anticancer Drugs and Metal Ions with DNA Base Pairs**
Ph.D Guide Name: Prof. P. Kolandaivel
Institute Name: Bharathiar University, Coimbatore, India

Post Doctoral Work :

Post Held: Postdoctoral Fellow,Duration: **March 2012 to April 2014 (2 years 2 months)**
Project: In silico Drug design, Halogen Bonding,
Advisor and Institution: **Pavel Hobza Group**, Department of Computational Chemistry,Institute of Organic Chemistry and Biochemistry , AS CR, v.v.i., Flemingovo nám. 2, CZ-166 10 Prague 6, Czech Republic.

Details of SLET/SET/NET passed, conducted by UGC/CSIR/Similar Tests accredited by the UGC

Name of the Eligibility Test	Subject	Month & Year of Passing
STATE ELIGIBILITY TEST FOR LECTURESHIP – (**SET**)	Physical Sciences	February 2016

Academic Qualifications

Degree/ Diploma	Subjects	Month & Year of passing	Name of Univ./Institution
SSLC	Maths, Science, Social Science	1998	Jaivabai MPL G HSS Tirupur
HSC	Physics, Chemistry, Biology, Maths	2000	St. Joseph Mat HSS Tirupur
Diploma in Microsoft Professional	M.S Windows, Linux, Fortran Programme	2000	Maha Computer, Tiruppur,
B.Sc Physics	Major: Physics Allied - Chemistry and Maths	2003	L.R.G Government Arts and Science College, Tiruppur, Bharathiar University, Coimbatore.
M.Sc Physics **(Gold Medal)**	Physics	2005	Nallamuthu Gounder Mahalingam College, Pollachi (Bharathiar University,Coimbatore).
M.Phil Physics	Physics	2007	Bharathiar University, Coimbatore, Tamilnadu
Ph.D Physics	Physics	2012	Bharathiar University, Coimbatore, Tamilnadu

Teaching Experience :

S. No	Positions held	Name of the Institutions	Duration		Years of Experience
			From	To	
1.	Temporary Assistant Professor	Manonmaniam Sundaranar University, Tirunelveli	23.07.2014	30.04. 2015	9 Months 8 days
2.	Temporary Assistant Professor	Manonmaniam Sundaranar University, Tirunelveli	23.07.2015	16.02. 2016	6 Months 25 days
3.	Young Scientist (DST-SERB)	Manonmaniam Sundaranar University, Tirunelveli	17.02. 2016	11.08.2019	3yrs 6 months

4	Temporary Assistant Professor	Manonmaniam Sundaranar University, Tirunelveli	02.08.2022	15.06.2023	9 months 15 days
5	Temporary Assistant Professor	Manonmaniam Sundaranar University, Tirunelveli	21.07.2023	Till date	9 months
Teaching and Research Experience					**5 Years 9 months**
6	Postdoctoral Fellow	Institute of Organic Chemistry and Biochemistry , Prague , Czech Republic	1.03.2012	30.04. 2014	2 years 2 months
Research Experience					**2 Years 2 months**
Total Experience					**7 Years 11 months**

Postdoctoral Fellow,Duration: **March 2012 to April 2014 (2 years 2 months)**

Project Awarded

1. Understanding the Potency of Inhibitors toward CK2 from Quantum Mechanics / Molecular Mechanics (QM/MM) and Molecular Dynamics (MD) study" under the scheme "**Start Up Research Grant (Young Scientist)**" under the DST - Science & Engineering Research Board (SERB) in the broad area of Physical and Mathematical Sciences, **File Number: YSS/2015/000275** at a total cost of **Rs. 31,53,993/- Duration 3 Years 6 months.**
2. Understanding the impact of halogen inhibitors in Histone deacetylases and the challenges in developing novel anticancer inhibitors: A QuantumMechanics (QM), Mol ecular Dynamics (MD), Chemical Synthesis and Bioassay study. June 2024, **File No.: DST/WISE-PDF/PM-67/2023,** Sanction Order- October 2024 , Total cost: **Rs 38,28,328/-, Duration: 3 Years**

Editor for Journal

1. Symbiosis- International Journal of Molecular and Theoretical Physics- **February 3rd 2017 onwards**

Reviewer for Journals

1. Physical Chemistry Chemical physics- 26th Nov 2015 onwards.
2. New Journal of Chemistry- 4th August 2015 onwards.
3. RSC advances, 9th Sep 2013 onwards.
4. Crystal Growth & Design- 2019 onwards.
5. Journal of Molecular Liquids- 2019 onwards.
6. Journal of Physical Organic Chemistry- 2020 onwards.

Organized Seminar/ Conference / Workshop

Secretary for the **Refresher Course on Physics (RCP – 2018)"** on 29th and 30th January 2018, Department of Physics, Manonmaniam Sundaranar University, Tirunelveli.

Resource Person

Resource Person in state level seminar on **Material science, 24 February 2023, Aditanar College Tiruchendur.** Invited talk entitled "An outlook of Emerging trends in Biomaterials" by **Palanisamy Deepa**.

Refresher Course on Physics

1. Participated in **Short Term Course on Faculty Empowerment programme on student success (FEPS- 2018)** held from 18- 24th January 2018 organised by Department of Education (DD & CE) Manonmaniam Sundaranar University, Tirunelveli.

Chair Session

1. International Conference on Molecular Spectroscopy (**ICMS 2017**)", Mahatma Gandhi University, Kottayam, Kerala, India, 8-10 December 2017.
2. National conference on Energy Materials (**NCEM-2018**), Department of Physics, Manonmaniam Sundaranar University, Tirunelveli, June 29-30 2018.
3. Second World Congress on Microscopy: Instrumentation, Techniques and Applications in Life Sciences and Materials Sciences (**WCM 2018**) on 10, 11 & 12 August 2018, Kottayam, Kerala, India**.**

Rapporteur

1. Newer Vistas to Animal Nutrition Research Towards Climate Resilient Animal Production for Livelihood, Food and Nutritional Security, **WANACON 2025**, January 20-22, 2025, Nagpur Veterinary college, Nagpur, India.

Invited Talk at International Conferences

1. Invited talk entitled "**Understanding the significance of Molecular Quantum Mechanics in Biomolecules"** at the **Second World Congress on Microscopy: Instrumentation, Techniques and Applications in Life Sciences and Materials Sciences (WCM 2018)** on **10, 11 & 12 August 2018, Kottayam, Kerala, India.**
2. Invited talk entitled "**Understanding the potency of Non-covalent interactions in Biomolecules**" at the "**International Conference on Molecular Spectroscopy**

(ICMS 2017)", Mahatma Gandhi University, Kottayam, Kerala, India, 8-10 December 2017

3. Invited talk entitled "Role **of computational Quantum Mechanics in Biomolecules**" at the **Advanced School and Workshop on Quantum Science and Quantum Technologies** held at the Abdus Salam International Centre for Theoretical Physics (ICTP), in Trieste , Italy from **04 September 2017 to 15 September 2017.**

Awards:

1. Fund provided by ICTP for accommodation and travel to participate and present a talk entitled " **Role of computational Quantum Mechanics in Biomolecules**" at the **Advanced School and Workshop on Quantum Science and Quantum Technologies** held at the Abdus Salam International Centre for Theoretical Physics (ICTP), in Trieste , Italy from **04 September 2017 to 15 September 2017.**
2. **Young Scientist award: February 2016 –2019**
3. **Qualified STATE ELIGIBILITY TEST FOR LECTURESHIP – (SET -2016) in Physical Sciences**
4. **Postdoctoral Fellow award March 2012 to April 2014**
5. Fund provided by ICTP for accommodation and travel to participate in the "**2nd Conference on Systems Biology and New Sequencing Techniques preceded by Introductory lectures on Quantitative Approaches to Biological Problems**" held at The Abdus Salam International centre for Theoretical Physics, 31st October - 4th November 2011, Miramare, Trieste, Italy.
6. **Senior Research Fellow Award** of Council of Scientific and Industrial Research, **(SRF-CSIR)** Government of India, Duration: April 2009-January 2012
7. **Gold medal** – 1st Rank Certificate in M. Sc Physics 2005.
8. **Proficiency Rank 1st** for Major subject Physics in B. Sc Physics 2003.
9. **Proficiency Rank 2nd** for Allied subject Maths in B. Sc Physics.
10. **First Class in Tamil Eligibility Certificate (Tamil) conducted by Tamil Teachers Association, 1998**.
11. Vivekananda Academy of Cultural Studies (VACS), Certificate of passing Indian Culture- 20.01.2002.
12. Vivekananda Academy of Cultural Studies Certificate Passed with First Class

(The Ramayana Our National Epic-12.1.2001).

13. Certificate From Gandhi Study Centre (My Experiments with Truth) Passed with First Class - 30.01.2001.

14. Balavikas Group II Certificate- Passed- August 4 1996.

Book Chapter-1

1. Michal Kolar, **Palanisamy Deepa,** Haresh Ajani, Adam Pecina and Pavel Hobza Characteristics of a σ-hole and the Nature of a Halogen Bond, **Book Title: Halogen Bonding II (Impacts on Materials Chemistry and Life Sciences), Top Curr Chem (Book Chapter**. ISSN-0340-1022, ISSN-1436-5049 (electronic), ISBN 978-3-319-15731-3, ISBN 978-3-319-15732-0 (eBook), Springer International Publishing Switzerland 2014, **)** 359, 2015, 1–26. **Impact Factor: 8.905, Citation: 9.**

List of Publications- International -32

1. Duraisamy Thirumeignanam , **Palanisamy Deepa**, Assessing the Mycobacterium Tuberculosis L, D-transpeptidase 2 binding strength with Carbapenem (T208) ligand and its modelled Halogen (Br, Cl, F) and non-Halogen (NH2 and SH) derivative Journal of Biomolecular Structure and Dynamics, **2025 (Under revision)**
2. **Palanisamy Deepa**, Duraisamy Thirumeignanam, Understanding the impact of Halogen Functional Group (Br, Cl, F, OH) in Amprenavir Ligand of the HIV Protease. Journal of Biomolecular Structure and Dynamics, 2023. 16:1-14 Impact Factor: **5.235**.
3. **Palanisamy Deepa** , Duraisamy Thirumeignanam, Understanding the impact of anticancer halogenated inhibitors and various functional groups (X = Cl, F, CF 3 , CH 3 , NH 2 , OH, H) of casein kinase 2 (CK2), **Journal of Biomolecular Structure & Dynamics**,11, **2022**, 5036-5052. **Impact Factor: 5.235.**
4. **Palanisamy Deepa** , Duraisamy Thirumeignanam, Rising trend on the halogen and non-halogen derivatives (Br, Cl, CF3, F, CH3 and NH2) in ruminal β-d-Xylopyranose – a quantum chemical perspective, **Journal of Biomolecular Structure and Dynamics**, 1, **2022**, 449-467. **Impact Factor: 5.235.**
5. **Palanisamy Deepa** , Duraisamy Thirumeignanam, Understanding the potency of malarial ligand (D44) in plasmodium FKBP35 and modelled halogen atom (Br, Cl,

F) functional groups**, Journal of Molecular Graphics and Modelling,** 97**, 2020,** 107553 **Impact Factor: 2.942**

6. **Palanisamy Deepa** A Quantum Chemical Perspective on the Potency of Electron Donors and Acceptors in Pnicogen bonds (AS...N, P...N, N...N), **Journal of Molecular Modeling**, 26, **2020,**11. **Impact Factor: 2.172**
7. **Palanisamy Deepa** Does the stability of the stacking motif surpass the planar motif in 2-amino-4-nitrophenol? — a CCSD(T) analysis, **Journal of Molecular Modeling, 2019,** 25:6 **Impact Factor: 2.172**
8. **Palanisamy Deepa**, D. Thirumeignanam, P. Kolandaivel. An overview about the impact of Hinge Region towards the Anticancer Binding Affinity of the Ck2 Ligands- A Quantum Chemical Analysis, **Journal of Biomolecular Structure and Dynamics**, 37, **2019**, 3859-3876.**Impact Factor: 5.235.**
9. G.Radha, B. Vijaya Pandiyan, P. **Deepa**, S. Govindarajan, P.Kolandaivel, and D. Nataraj, Synthesis and experimental studies on supramolecular synthons of aminoguanidinium carboxylates - A case Study of π-hole bonded carbon bonding via theoretical approaches, **Chemistry Select** 3, **2018,** 10032-10048**. Impact Factor: 2.307**
10. Subramaniam Kavitha, **Palanisamy Deepa**, Mylsamy Karthika, Ramasamy Kanakaraju, Hybrid DFT Study on non-covalent interactions and their influence on pK_a's of magnesium-carboxylate complexes, **Journal of Molecular Graphics and Modelling.** 85, **2018**, 13e24 **Impact Factor: 2.942**
11. **Palanisamy Deepa, B.Vijaya Pandiyan and Ponmalai Kolandaivel,** Does the presence of Water Clusters induce the binding affinity of CK2 Halogen Ligands? – A Quantum Chemical Perspective Study**, International Journal of Quantum Chemistry,** 118, **2018,** e25644**. Impact Factor: 2.437**
12. **Palanisamy Deepa** Understanding the nature of Metal Oxalato Complexes with Purine Nucleobase- A Quantum Chemical Approach. **International Journal of Molecular and Theoretical Physics,** 1, **2017,** 1-10**.**
13. **Palanisamy Deepa**, B. Vijaya Pandiyan, Duraisamy Thirumeignanam, Ponmalai. Kolandaivel, Understanding the potency of fatty acids with bovine β lactoglobulin - A Quantum Chemical Approach, **Journal of Molecular Graphics and Modelling**, 74, **2017**, 105-116. **Impact Factor: 2.942**

14. **Palanisamy Deepa**, An Overview about the Factors Influencing CK2 Ligands and the Impact of Crystal Waters - A Theoretical Study, **Crystal Growth and design**, 17, **2017**, 1299- 1315, **Impact Factor: 4.01**.
15. B. Vijaya Pandiyan, **P. Deepa,** and P. Kolandaivel, How do halogen bonds (S– O···I, N–O···I and C–O···I) and halogen–halogen contacts (C–I···I–C, C–F···F–C) subsist in crystal structures? A quantum chemical insight, **Journal of Molecular Modeling,** 23, **2017,**16. **Impact Factor: 2.172**.
16. B. Vijaya Pandiyan, **P. Deepa**, and P. Kolandaivel, Studies on the σ –hole bonds (halogen, chalcogen,pnicogen and carbon bonds) based on the orientation of crystal structure, **Molecular Physics,** 114, **2016**, 3629-3642. **Impact Factor: 1.937.**
17. Subramaniam Kavitha, **Palanisamy Deepa**, Mylsamy Karthika, Ramasamy Kanakaraju, Topological analysis of Metal - Ligand and Hydrogen bonds in the first row transition metal hybrid structures - A Computational study, **Polyhedron,** 115, **2016**, 193-203. **Impact Factor: 2.975.**
18. B. Vijaya Pandiyan, **P. Deepa,** and P. Kolandaivel**,** Does the occurrence of resonance (by the delocalization of radical / cationic /anionic charges) induce the existences of intra molecular halogen --- halogen contacts?, **RSC Advances**, 6, **2016**, 66870. **Impact Factor: 4.036.**
19. B. Vijaya Pandiyan, **P. Deepa,** and P. Kolandaivel**,** Do resonance-assisted intramolecular halogen bonds exist without a charge transfer and a r-hole?, **Physical Chemistry Chemical Physics**, 17, **2015**, 27496-27508. **Impact Factor: 3.945.**
20. B. Vijaya Pandiyan, **P. Deepa,** and P. Kolandaivel**,** On the Nature of Non- Covalent Interactions in 2,5-Dichloro-1,4 Benzoquinone Isomers – Ground- and Excited-State Properties **Physical Chemistry Chemical Physics**, 16, **2014,** 19928-19940. **Impact Factor: 3.945.**
21. **P. Deepa**, R. Vijay Solomon, S. Angeline Vedha, P. Kolandaivel, P.Venuvanalingam, The Nature of Hydrogen Bonding in $R_2^2(8)$ crystal motifs– A Computational Exploration, **Molecular Physics,**112, **2014,** 3195-3205. **Impact Factor: 1.937.**

22. Robert Sedlak, **Palanisamy Deepa** and Pavel Hobza, Why is the L-shaped structure of $X_2..X_2$ (X= F, Cl, Br, I) complexes more stable than other structures? **Journal of Physical Chemistry A**, 118**, 2014**, 3846-3855. **Impact Factor: 2.944**.
23. **Palanisamy Deepa**, Robert Sedlak and Pavel Hobza, On the origin of the substantial stabilisation of the electron-donor 1,3-dithiole-2-thione-4-carboxyclic acid...I_2 and DABCO...I_2 complexes, **Physical Chemistry Chemical Physics**, 16, **2014**, 6679-6686, **Impact Factor: 3.945**
24. **P. Deepa**, B. Vijaya Pandiyan, P. Kolandaivel, and Pavel Hobza, Halogen Bonds in Crystal TTF derivatives: An Ab Initio Quantum Mechanical Study, **Physical Chemistry Chemical Physics**, 16, **2014,** 2038-2047. **Impact Factor: 3.945.**
25. B. Vijaya Pandiyan, P. Kolandaivel and **P. Deepa,** A Theoretical Perspective of the Nature of Hydrogen-Bond types – the Atoms in Molecules Approach, **Molecular Physics**, 112, **2014,** 1609-1623. **Impact Factor: 1.937**.
26. **P. Deepa** , P. Kolandaivel and K. Senthilkumar, Structural properties and the effect of platinum drugs with DNA base pairs, **Structural Chemistry,** 24, **2013,** 583-595. **Impact Factor: 1.795.**
27. **P. Deepa**, P. Kolandaivel and K. Senthilkumar, Theoretical investigation of interaction between Psoralen and Altretamine with stacked DNA base pairs, **Materials Science and Engineering C-Materials For Biological Applications,** 32, **2012**, 423-431. **Impact Factor: 7.9.**
28. **P. Deepa,** P. Kolandaivel and K. Senthilkumar, Hydrogen bonding studies of Amino acid side chains with DNA base pairs, **Molecular Physics**, 109, **2011**, 1995-2008. **Impact Factor: 1.937.**
29. **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-tetrad and SG-tetrads, ***Computational and Theoretical Chemistry*** **,** 974, **2011**, 57-65. **Impact Factor: 2.292.**
30. **P. Deepa**, P. Kolandaivel and K. Senthilkumar, First and second coordination spheres in 8-azaxanthinato salts of divalent metal aquacomplexes – Ab initio and DFT study, **Polyhderon**, 30, **2011,** 1431. **Impact Factor: 2.975.**
31. **P. Deepa**, P. Kolandaivel and K. Senthilkumar, Structural Properties and the Effect of 2,6-Diaminoanthraquinone on G-Tetrad, Non-G-Tetrads, and Mixed

Tetrads-A Density Functional Theory Study, **International Journal of Quantum Chemistry**, 111, **2011,** 3239. **Impact Factor: 2.437**.

32. **P. Deepa**, P. Kolandaivel and K. Senthilkumar, Interactions of anticancer drugs with usual and mismatch base pairs - Density functional theory studies, **Biophysical Chemistry**, 136, **2008**, 50-58. **Impact Factor: 3.8**.
33. **P. Deepa** and P. Kolandaivel, Studies on Tautomeric Forms of Guanine-Cytosine Base Pairs of Nucleic Acids and Their Interactions with Water Molecules, **Journal of Biomolecular Structure & Dynamics**. 25, **2008,** 733-746. **Impact Factor: 5.235.**

List of Publications- National

1. **Palanisamy Deepa**, Duraisamy Thirumeignanam entitled "**Quantum Chemical Perspective on the Nature of Valine Dipeptide –A Potential Energy Surface Study**" in the conference on "Proceedings International Workshop on Advanced Materials and Devices", ISBN:978-93-81402-38-2, January 8 to 12, 2017.

International conferences/ Summer School and Seminar Participated/ Presented Paper in Foreign Nationals

1. **Palanisamy Deepa, Jindrich Fanfrlík, Agnieszka K. Bronowska, Jan Rezac, Aneta Kadlcikova, Pavel Majer, Vladimir Krystof, Martin Lepsik, Pavel Hobza,** presented paper entitled **"Quantum Chemistry based Docking and Scoring for Design of Protein Kinase Inhibitors**", in the conference on "**VIII congress of the International Society of Theoretical Chemical Physics" held at** ISTCP, Budapest, Hungary, 25-31st August 2013.
2. **Deepa Palanisamy**, Jindrich Fanfrlik, Pathik S. Brahmkshatriya, Jiri Brynda, Petr Cankar, Vladimir Krysto, Jan Rezac, Martin Lepsik, and Pavel Hobza, Presented paper entitled "**Understanding the potency of competitive CDK2 inhibitors using quantum chemical scoring" in the conference on "International Congress on Natural Anticancer Drugs**" held at Palacky University, Olomouc, Czech Republic, 30th June -July 4th 2012.
3. Actively participated in the "**2nd Conference on Systems Biology and New Sequencing Techniques preceded by Introductory lectures on Quantitative Approaches to Biological Problems**" held at The Abdus Salam International centre for Theoretical Physics, 31st October - 4th November 2011, Miramare, Trieste, Italy.

International conferences/ Summer School and Seminar Participated/ Presented Paper in India

1. Presented paper **Palanisamy Deepa,** Duraisamy Thirumeignanam, Balasubramanian Sundarakannan, **Understanding the Potency of strength of Various Fatty Acids in Bovine Lactoglobulin – a Biomolecular Approach,** Oral presentation, Newer Vistas to Animal Nutrition Research Towards Climate Resilient Animal Production for Livelihood, Food and Nutritional Security, **WANACON 2025**, January 20-22, 2025, Nagpur Veterinary college, Nagpur, India.
2. Presented paper **Palanisamy Deepa,** Duraisamy Thirumeignanam, "**Understanding the potency of 2(S)-AMINO-6-ORONOHEXANOIC acid in Plasmodium Falciparum Arginase and modelled Halogen Atom Functional Groups**", Oral presentation – ICCMIA, 27 and 28th January2023, MS University, Tirunelveli.
3. Presented paper M.Mohanaraghavan, R. Sivagurusundar, **Dr. P. Deepa***, Dr. G. Annadurai*, **Construction of novel n-type semiconductor anchor on 2D rod like FeMoO4/chitosan/CdO for visible light driven photocatalytic degradation of Norfloxacin**, ICEBB, 9 and 10th March 2023, MS University, Tirunelveli.
4. Presented paper Ajayvasanth S , Madhumitha , Amutha E , **Deepa P** *, Annadurai G*. **Preparation and characterization of tin oxide nanoparticles via the Co-precipitation method**. ICEBB, 9 and 10th March 2023 MS University, Tirunelveli.
5. Presented paper V.Vinisha, **Dr. P. Deepa***, Dr. D. Thirumeignanam, **Analysing the Role of Potent Inhibitor (2-2'-Biphenyl-3,5-Diyldiacetic Acid) of Dengue Polymerase – A Quantum Mechanical Approach**, ICEBB, 9 and 10th March 2023 MS University, Tirunelveli.
6. Presented paper M. Sakthi, **Dr. P. Deepa***, Dr. D. Thirumeignanam**, Understanding the Impact of Inhibitor AMG 176 in (MCL1) Myeloid Leukemia Protein - A Quantum Mechanical Approach**. ICEBB, 9 and 10th March 2023 MS University, Tirunelveli.
7. Presented paper **Palanisamy Deepa**, Duraisamy Thirumeignanam entitled "**Quantum Chemical Perspective on the Nature of Valine Dipeptide –A Potential Energy Surface Study**" in the conference on "**Proceedings International Workshop on Advanced Materials and Devices**" held at Manonmaniam Sundaranar University, Tirunelveli on January 8 to 12, 2017.

ISBN:978-93-81402-38-2.

8. Presented paper **P. Deepa,** B. Vijaya Pandiyan and P. Kolandaivel entitled "**Characteristic Properties of Pnicogen Bonds- A Quantum Chemical Study**" in the conference on "**Asian Consortium on Computational Materials Science Theme Meeting on First Principles Analysis & Experiment: Role in Energy Research**" held at SRM University, Chennai on September 22 to 24, 2016. **ISBN:978-81-930475-5-2.**
9. Presented paper in seminar entitled "**Intercalation of Platinum drugs with stacked DNA base pairs"** in the **Theoretical Chemistry Symposium**, Indian Institute of Technology Kanpur, India, 8-12th December, 2010.
10. Presented paper in seminar entitled "**Theoretical study of the second coordination sphere in 8-azaxanthinato salts of divalent metal aquacomplexes**" in the **International Symposium** "**Of Molecules and Materials (A survey of Recent Concepts)" (OMAM)**, organized by the Indian Institute of science Education & Research, Kolkata, India, 28-29th December 2009.
11. Presented paper in seminar entitled "**Theoretical studies on drug and DNA binding mode**" in the **Discussion Meeting on Theoretical Chemistry** conducted by Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore and Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India, 18-22nd January, 2009.
12. Actively participated in the seminar in the **Theoretical Chemistry Symposium** conducted by **Bharathidasan** University, Tiruchirappalli, Tamilnadu, India, December, 2006.

National conferences/ Summer School/Workshop and Seminar Participated/ Presented Paper

1. Actively Participated in **A One Day Training on Preparation of Revised Bloom's Taxonomy Based Internal And Semester Exam Question Papers**, 24th January 2023 held at Manonmaniam Sundaranar University, Tirunelveli
2. Actively Participated in **A One Day Workshop on Intellectual Property Rights**, 15th February 2023 held at Manonmaniam Sundaranar University, Tirunelveli
3. Actively Participated in **Webinar on chemistry and Biology of Natural Products** on 24-25th July 2020 organized by CSIR-NEIST,Jorhat,Assam,India

4. Actively Participated in the workshop "**Science Academies' Lecture Workshop on Developments in Chemistry**" on 5-6th July 2018 organized by Department of Pharmaceutical Chemistry held at Manonmaniam Sundaranar University, Tirunelveli
5. Actively Participated in the workshop "***Computer Aided Drug Designing***" held during 13th -17th February 2017 at **Bioinformatics Centre & ARIS Cell, Madras Veterinary College**, Chennai – 600 007
6. Presented paper in seminar entitled S.Kavitha, **P.Deepa,** M.Karthika, R. Kanakaraju **"Computational analysis of Topological Parameters in Transition metal Organic - Inorganic Hybrid Materials"** at National Conference On Computational And Experimental Physics Of Functional Materials (**NCCEPFM-2016**), Namakkal, Tamil Nadu, India
7. Actively participated in the national seminar entitled "**Radiation Technology in Health Care and its Safety"** by Bharathiar University, Coimbatore India, 16-17th March, 2011.
8. Actively participated in the ICTS School on "**Understanding Molecular Simulations: Theory and Applications**" (ums 2010), Indian Institute of Technology Kanpur, India, November 04 -November 13, 2010.
9. Participated in Seminar on Nuclear Energy for National Development (NEND), Bhabha Atomic Research Centre, Mumbai and Department of Physics, Bharathiar University, Coimbatore, 2nd December 2009.
10. Actively participated in the Short term course on "**Photophysics of Organic systems: Theory and applications"** organized by Bharathiar University, Coimbatore, India, Indian Institute of Science, Bangalore and Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India, 1-4th February, 2006.
11. Actively participated in the National level seminar **on "Lasers in Technological and Biomedical Applications"** organized by the Department of Physics, St. Joseph's College (Autonomous), Tiruchirappalli, 27-28th January 2005.
12. Actively participated in the Awareness Programme on "**Applications of Radioisotopes and Radiation Technology for societal Development"** organized by Anna University, Chennai, 13-14th July 2004.
13. Actively participated in the UGC sponsored state level seminar on "**Super Ionic Conductors and its Applications –SICAA 2004"** organized by the Department of

Physics, Sri G.V.G.Visalakshi College for Women, Udumalpet, 18-19th September, 2004.

14. Actively participated in the National level seminar **on "VHDL Tools for VLSI Design**" sponsored by UGC**,** organized by Department of Electronics, PSG College of arts and science, Coimbatore, 18-19th September, 2003.
15. Actively participated in the state level seminar on "**Recent Developments in Physics and Communication"** organized by the Department of Physics, Maharaja College for Women, Perundurai, January 28, 2003.
16. Actively participated in the "**Value Education Training Camp**" organized by PSG College of arts and science, Coimbatore, 01.02.2003.

Member of Organizing Committee in Seminar/ Conference / Workshop

1. **National conference on Energy Materials (NCEM-2018)**, Department of Physics, Manonmaniam Sundaranar University, Tirunelveli, June 29-30 2018, (Organising Committee Member) .
2. **International Workshop on Advanced Functional Materials and Devices – IWAFMD2017**, Department of Physics, Manonmaniam Sundaranar University, Tirunelveli, January 8 -12, 2017. (Organising Committee Member) (Reception, compiring, invited talk, sessions and hall arrangement in charge of conference).
3. **Workshop on current trends in Emerging Materials for Technological Applications**, 18th August 2017, Department of Physics, Manonmaniam Sundaranar University, Tirunelveli, (Organising Committee Member).
4. **Sixth National Seminar on Advances in Materials Science (NSAMS-2017)**, Department of Physics, Manonmaniam Sundaranar University, Tirunelveli, March 2, 3-2017, (Organising Committee Member).
5. Open House Day of Department of Physics, Manonmaniam Sundaranar University, Tirunelveli, 3.11.2016, and conducted Rapid Examination and Quiz Programme for student participant.
6. **Fifth National Seminar on Advances in Materials Science (NSAMS-2014),** Department of Physics, Manonmaniam Sundaranar University, Tirunelveli, September 28-29, 2014. (Organising Committee Member).

Extension Activities

1. **Library In-charge** Of Department of Physics, , Manonmaniam Sundaranar

University, Tirunelveli, 2016- 2019
2. Mentor
3. I.M.Sc Course Teacher, Department of Physics, Manonmaniam Sundaranar University, Tirunelveli 2017- 2019.
4. Physics weekly Seminar Organizing Secretary 2009-2010, Department of Physics, Bharathiar University, Coimbatore.
5. Hostel Secretary 2009-2011, Bharathiar University, Coimbatore.
6. Member of National Service Scheme (NSS) -2001-2002.
7. National Service Scheme -(NSS) Special Camp Participation Certificate – 2-1-2002 to 11-1-2002.

PG Dessertation Completed
M.Sc Physics

1. M.Ahamed Abulaise Reg. No. 20224012521102, Understanding the impact of Halogen Drugs through drug Repurposing – A Quantum Mechanical Study, Survey and Experimental analysis
2. S.BOOMIKA, Reg.no. 20224012521108, Understanding the Impact of Medicinal Herbs (Phyllanthus emblica, Azadirachta indica and Murraya koeingi) for Drug Repurposing – A Comparative Analysis.
3. A. Daniel Reg. No. 20224012521111, Understanding the impact of Sulfa Drugs through drug Repurposing – A Quantum Mechanical Study, Survey and Experimental analysis
4. M.Karthikeyan Reg. No. 20224012521120, Understanding the impact of Amine Drugs through drug Repurposing – A Quantum Mechanical Study, Survey and Experimental analysis
5. S.KOHILA. Reg. No. 20224012521122, Understanding the impact of cancer drugs through drug Repurposing – A Quantum Mechanical Study, Survey and Experimental analysis
6. Mariselvam Reg. No. 20224012521125, Understanding the impact of Carboxylic acid Drugs through drug Repurposing – A Quantum Mechanical Study, Survey and Experimental analysis
7. Thanarubene Reg. No. 20224012521136, Understanding the impact of Alzheimer's Disease Drugs through drug Repurposing – A Quantum Mechanical Study, Survey and Experimental analysis
8. Photocatalytic Degradation of Rhodamine Using Co-Zno Nanoparticles Prepared By Simple Co-Precipitation Method. Student: S. Ajay vasanth, Reg No : 20214012521106, (2023).
9. Synthesis and Characterization of Nb2o5 Based Ternary composites For Photocatalytic Applications Student: M.Mohanaraghavan, Reg No : 20214012521122,(2023).
10. M.Sakthi - Understanding The Impact of Inhibitor Amg 176 In (Mcl1) Myeloid Leukemia Protein - A Quantum Mechanical Approach. Student: Reg. No. 20214012521135, (2023).
11. Analyzing The Role of Potent Inhibitor (2-2'-Biphenyl-3,5- Diyldiacetic Acid) Of Dengue Polymerase – A Quantum Mechanical Approach Student:V. Vinisha Reg. No. 20214012521148.
12. Strutural Properties and Binding analysis of Amprenavir with HIV-1 Protease - Molecular Quantum Mechanics Study , Student: J.Angel Asha, Reg.No: 20174012521102, (2019).
13. Strutural Properties and Binding analysis of 2(S)-Amino-6-Boronohexanoci acid with plasmodium Falciparum Arginase -Molecular Quantum Mechanics Study , Student: I.

Chitra, Reg.No: 20174012521105 (2019)**.**

14. Strutural Properties and Binding analysis of Carbapenem with Pencillin Binding Protein -Molecular Quantum Mechanics Study , Student: Mohaned Anees Fathima, Reg.No: 20174012521109 (2019)**.**
15. Strutural Properties and Binding analysis of Inositol Hexakisphosphate with Protein Tyrosine Phosphatase -Molecular Quantum Mechanics Study , Student: R.Monika, Reg.No: 20174012521110 (2019)**.**
16. Strutural Properties and Binding analysis of D44 with Plasmodium FKBP35 - Molecular Quantum Mechanics Study, Student: S.Sruthi, Reg.No: 20174012521123 (2019)**.**

Integrated. M.Sc Physics Dessertation Completed

1. Molecular Quantum Mechanics Study on the structural Properties of Anticancer Drug (Cryptolepine)- DNA Binding , Student: P.Kiruthika, S.Lavanya,C.Santhiya Bharathi (2019)**.**, Reg. No: 361203, 361204, 361208**.**

2. Molecular Quantum Mechanics Study on the structural Properties of Anticancer Drug (Ellipticine)- DNA Binding , Student: P.T.Nisha, K.Ranjitha, U.K.Mohamed Irshath (2019)**.**, Reg. No: 361206, 361207, 361219

Internship Mentor

Int M.Sc Physics (2023)

1. BALA B
2. GUNA M
3. MANJU S
4. RAHUL RV
5. SURESH E

Int M.Sc Physics (2024)

6. ESAKKIMUTHU .M
7. JAYAKUMAR K
8. MUKILAN SURJITH P
9. SAKTHI SABARI S
10. VASANTH S

Extra Curricular activities

S No.	Type of Skill	Nature of Proficiency
1	Member of National Service Scheme (NSS) 2001-2002.	NSS
2	National Service Scheme -(NSS) Special Camp -2-1-2002 to 11-1-2002.	Participation Certificate
3	Winner in Throw Ball, Mano Day Sports Competitions 2017-2018, Ms University.	Merit Certificate
4	Winner in Chess, Mano Day Sports Competitions 2017-2018, Ms University.	Merit Certificate
5	Runner in Tennikoit, Mano Day Sports Competitions 2017-2018, Ms University.	Merit Certificate
6	First prize in Running (100 mts) at International Women's Day celebrations 2018 , MS university.	Certificate of Appreciation

7	Second prize in Poem at International Women's Day celebrations 2018 , MS university.	Certificate of Appreciation
8	Second prize in Badminton at International Women's Day celebrations 2018 , MS university.	Certificate of Appreciation
9	Second prize in Tennikoit at International Women's Day celebrations 2018 , MS university.	Certificate of Appreciation
10	Winner in Throw Ball at International Women's Day celebrations 2018, MS university.	Certificate of Appreciation
11	Awarded Participation Chess Competition Certificate for Students Associations Campus Competitions 2009,Bharathiar University	Certificate of Appreciation
12	Winner in CARROM for Athletics in LRG Govt.Arts College (04/03/2003)	Certificate of Appreciation

13	Physics 2nd Year Class Representative 2002 in LRG Govt.Arts College.	Certificate of Appreciation
14	Second Prize for Tamil Oratorical Competition with certificate of merit (1994-1995).	Certificate of Appreciation
15	Indian Culture and Spiritual Training Camp, organized by Sri Sathya Sai Seva Organization, Tiruppur- December 1993.	Certificate of Appreciation
16	Third prize in Group Song (2001-2002) with Certificate for Performing arts in LRG Govt.Arts College.	Certificate of Appreciation
17	Actively Participated in Indian Culture and Spiritual Courses for High School Student, by Sri Sathya Sai Seva Organizations, Tiruppur- December 28.12.1997.	Certificate of Appreciation

Declaration

I certify that to the best of my knowledge and belief the particulars given above are correct.

(Dr.P.Deepa)