

CURRICULUM VITAE

Dr. RENJITH R.

Assistant Professor,

Department of Physics,

Government College, Kasargod, Kerala, India

Mobile: +91 82 81 56 01 52

Email: renjithkadavoor@gmail.com; drrenjith@universitycollege.ac.in

ResearcherID:E-7342-2016

Google Scholar: <https://scholar.google.co.in/citations?user=5Xrgrv4AAAAJ&hl=en>

RESEARCH INTERESTS

- Molecular Modeling
- Simulation of material properties using Quantum Chemical Methods.
- Molecular Dynamics
- Molecular Docking and QSAR studies

RESEARCH EXPERTISE

- Computational materials and molecular modeling: ab initio, molecular dynamics, molecular docking
- Experience in following codes and program packages: Gaussian, Schrödinger Materials Science Suite (Jaguar, Desmond, MacroModel, Canvas, Maestro), Quantum Wise/Synopsis ATK, SCM ADF, GAMESS, Quantum Espresso, Autodock Vina, Multiwfn, VMD, ORCA, etc.

COMPUTATIONAL SKILLS

- Linux and windows operating systems
- Expertise in Gaussian16 software for Quantum chemistry calculations.

EDUCATION

- 01 March 2016 Doctor of Philosophy (Ph.D.), University of Kerala, Trivandrum, Kerala, India.
Dissertation Title: Spectroscopic Investigations of certain Azatricyclo and Anthraquinone Derivatives.
- 2010 Master of Science (M.Sc.) Physics, University of Kerala, Trivandrum, Kerala, India.
- 2008 Bachelor of Science (B.Sc.) Physics, University of Kerala, Trivandrum, Kerala, India.

TEACHING EXPERIENCE

UG and PG – 07 years

TEACHING POSITIONS

- 2023 onwards Assistant Professor, Department of Physics, Government College, Kasargod, Kerala, India.
- 2021 – 2023 Assistant Professor, Department of Physics, University College, Thiruvananthapuram, Kerala, India.
- 2019 – 2021 Assistant Professor of Physics, Central Polytechnic College, Vattiyoorkavu, Trivandrum, Kerala, India.
- 2017-2019 Assistant Professor, DST-FIST funded P.G. Department of Physics, T.K.M. College of Arts and Science, Kollam, Kerala, India.
- 2016-2017 UGC FDP Guest Lecturer, S.N. College, Varkala, Trivandrum, Kerala, India.

AWARDS AND HONORS

- 2011 Qualified Graduate Aptitude Test in Engineering, India.
- 2011 CSIR-UGC Junior Research Fellowship, India.
- 2014 CSIR-UGC Senior Research Fellow.

RESEARCH SUPERVISION

Research Guide at University of Kerala (PHYSICS)

- Ph.D. 4 (Completed – Nil. Ongoing – 4)
- M.Sc. Project 15

ORGANIZATIONAL PERFORMANCES

- 2019 **District Coordinator**, Sasthrapadham-2019, Samagra Shiksha, Kerala.
- 2019 **District Coordinator**, Sasthrajalakam-2019, SIET, Kerala.
- 2019 **Judge**, State Science Fair, Kerala.

COURSES/WORKSHOPS ATTENDED

- 2013 Science Academies' Refresher Course in Quantum Mechanics, held at JSS Institutions Campus, Suttur, Mysore, Karnataka, India.
- 2018 Induction Programme for College Teachers held at IISER, Pune, Maharashtra, India.
- 2020 Online Refresher Course in Material Science held at University of Kerala, Trivandrum, Kerala, India.
- 2020 International e-Workshop on "Docking, QSAR and Molecular Dynamics" jointly organized by Department of Biotechnology, Ramaiah Institute of Technology and Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ramaiah University of Applied Sciences, Bengaluru, Karnataka, India in association with IEEE-EMB MSRIT student chapter and SRIGEN-Society of Biotechnologists.
- 2020 Faculty Development Programme from 2020-05-25 to 2020-05-29 on Moodle Learning Management System organized by Sree Narayana College, Chengannur and training is offered by the Spoken Tutorial Project, IIT Bombay, funded by the National Mission on Education through ICT, MHRD, Govt. of India.
- 2021 AICTE Training and Learning (ATAL) Academy Online Elementary FDP on " "Drug Engineering through Computer Aided Drug Design"" at Dr. HARISINGH GOUR CENTRAL UNIVERSITY SAGAR M.P.
- 2021 Short term course on "Materials Characterization Techniques" conducted as a part of quality improvement program, organized by the Department of MEMS, IIT Indore.

- 2021 Online FDP on "Engineering Pedagogy in the Covid 19 Pandemic Scenario" organized by Government Polytechnic College Chelakkara Thrissur funded by Department of Technical Education, Kerala.
- 2022 Online Refresher Course on Material Science conducted by HRDC, University of Kerala, Thiruvananthapuram.

PAPER PRESENTATIONS IN CONFERENCES

1. Dr. Renjith R., presented a paper titled **Theoretical Investigation on the Reactivity Descriptors of Novel Benzimidazole-Oxadiazole Derivatives** in the **International Conference on 'Engrossing Trends in Chemistry'** organized by PG Department of Polymer Chemistry in association with IQAC, Govt. college Attingal from December 01-03 2021(online)

RESEARCH PUBLICATIONS

Journal Papers 34 (26 International + 8 National)

Google Scholar

Citations: 403

h-index: 12

Verified Pre-publication reviews: 35 (Elsevier Database)

International Publications

1. Exploring the structural, photophysical and optoelectronic properties of a diaryl heptanoid curcumin derivative and identification as a SARS-COV-2 inhibitor, V.P. Archana, S.J. Armakovic, S. Armakovic, I. Celik, J.B. Bhagyasree, K.V. Dinesh Babu, M. Rudrapal, I.S. Divya, Renjith Raveendran Pillai, J. Mol. Struct. 1281 (2023) 135110 <https://doi.org/10.1016/j.molstruc.2023.135110>.
2. Synthesis and investigations of reactive properties, photophysical properties and biological activities of a pyrazole-triazole hybrid molecule, Khalid Karrouchi, Ismail Celik, Saad Fettach, T. Karthick, Khalid Bougrin, Smaail Radi, My El Abbes Faouzi, M'hammed Ansar, R. Renjith, Journal of Molecular Structure, 1265 (2022) 133363 <https://doi.org/10.1016/j.molstruc.2022.133363>
3. Synthesis, molecular modeling, quantum mechanical calculations and ADME estimation studies of benzimidazole-oxadiazole derivatives as potent antifungal agents, U.A. Cevik, I. Celik, A. Isik, Renjith Raveendran Pillai, T.E. Tallei, R. Yadav, Y. Ozkay, Z.A. Kaplancikli, Journal of Molecular Structure, 1252 (2022) 132095 <https://doi.org/10.1016/j.molstruc.2021.132095> (Impact Factor - 3.196)
4. Structural, spectroscopic, and in silico studies of 3-(dimethylamino)-1-(thiophen-2-yl)propan-1-ol: A potential antidepressant agent, Nuthalapati Poojith, Madhuprasad Kigga, J. John Rose, Krishna Murthy Potla, Suneetha Vankayalapati, Sampath Chinnam, Suchetan Parameshwar Adimoole, Renjith Raveendran Pillai, Journal of Molecular Structure, 1250 (2022) 131859 <https://doi.org/10.1016/j.molstruc.2021.131859> (Impact Factor - 3.196)

5. Investigation of Pharmaceutical Importance of 2H-Pyran-2-One Analogues via Computational Approaches, S.E. Shetgaonker, S.P. Kollur, **Renjith Raveendran Pillai**, T. Karthick, S.J. Armakovic, S. Armakovic, C. Shivamallu, R.G. Amachawadi, A. Syed, A.M. Elgorban, A.H. Bahkali, F.V. Singh, *Symmetry* 13 (2021) 1619, <https://doi.org/10.3390/sym13091619> (Impact Factor – 2.713)
6. An analysis of structural, spectroscopic, quantum chemical and in silico studies of ethyl 3-[(pyridine-2-yl)amino]propanoate: A potential thrombin inhibitor, Nuthalapati Poojith, Nannapaneni Usha Rani, Krishna Murthy Potla, J. John Rose, P.A. Suchetan, **Renjith Raveendran Pillai**, Suneetha Vankayalapati, *Journal of Molecular Structure*, 2020 (1226) 129378, <https://doi.org/10.1016/j.molstruc.2020.129378> (Impact Factor – 3.196)
7. Indole moiety induced biological potency in pseudo-peptides derived from 2-amino-2-(1H-indole-2-yl) based acetamides: Chemical synthesis, in vitro anticancer activity and theoretical studies, Kollur Shiva Prasad, **Renjith Raveendran Pillai**, Madhav Prasad Ghimire, Rajyavardhan Ray, Manual Richter, Chandran Shivamallu, Anisha S. Jain, Shashanka K. Prasad, Sushma P., Stevan Armakovic, Sanja J. Armakovic, Raghavendra G. Amachawadi, *Journal of Molecular Structure*, 2020 (1217) 128445, <https://doi.org/10.1016/j.molstruc.2020.128445> (Impact Factor – 3.196)
8. Tumoricidal Potential of Novel Amino-1,10-phenanthroline Derived Imine Ligands: Chemical Preparation, Structure, and Biological Investigations, Kollur Shiva Prasad, **Renjith Raveendran Pillai**, Chandan Shivamallu, Shashaka K. Prasad, Anisha S. Jain, Sushma Pradeep, Stevan Armakovic, Sanja J. Armakovic, Chandrashekar Srinivasa, Sharadadevi Kallimani, Raghavendra G. Amachawadi, Veena Malligere Ankegowada, Najat Marraiki, Abdallah M. Elgorban, Asad Syed, *Molecules*, 2020 (25) 2865, <https://doi.org/10.3390/molecules25122865> (Impact Factor: 4.412)
9. Synthesis, Hirshfeld Surface Analysis and DFT Studies of Ethano-tetracyclic Tetracene Derivatives, Mujeeb A. Sulthan, Hazem A. Ghabbour, Saied M. Soloman, **Renjith Raveendran Pillai**, Mansour S. A. Galil, *Journal of Chemical Crystallography*, 2020, 196-204, <https://doi.org/10.1007/s10870-020-00841-6> (Impact Factor: 0.603)
10. Photophysical properties and theoretical investigations of newly synthesized pyrene-naphthalene based Schiff base ligand and its copper(II) complexes, Kollur Shiva Prasad, **Renjith Raveendran Pillai**, Stevan Armakovic, Sanja J. Armakovic, *Inorganica Chimica*

Acta, ISSN/eISSN:0020-1693/1873-3255 486 (2019) 698-703.
<https://doi.org/10.1016/j.ica.2018.11.045> (Impact Factor: 2.545).

11. Synthesis, Spectroscopic Characterization, reactive properties by DFT calculations, molecular dynamics simulations and biological evaluations of Schiff bases tethered 1,2,4-triazole and pyrazole rings, **Renjith Raveendran Pillai**, Khalid Karrouchi, Saad Fettach, Stevan Armakovic, Sanja J. Armakovic, Younes Brik, Jamal Taoufik, Smaail Radi, My El Abbes, Faouzi Mohammed Ansar, Journal of Molecular Structure, 1177 (2019) 47-54.
<https://doi.org/10.1016/j.molstruc.2018.09.037>. (Impact Factor : 3.196)
12. Remarkable colorimetric sensing behaviour of pyrazole-based chemosensor towards Cu(II) ion detection: synthesis, characterization and theoretical investigations, N. Nayak, K.S. Prasad, **Renjith Raveendran Pillai**, Stevan Armakovic, Sanja J. Armakovic, RSC advances, 8 (2018) 18023-18029. <http://dx.doi.org/10.1039/C8RA02905A>. (Impact factor: 3.361).
13. Theoretical Investigation on the reactivity and photophysical properties of cobalt(II) and manganese(II) complexes constructed using Schiff base ligands based on ALIE and TDDFT calculations, K.S. Prasad, **Renjith Raveendran Pillai**, S. Armakovic, S.J. Armakovic, Polyhedron, ISSN:0277-5387, (2017), 129, 141-148,
<https://doi.org/10.1016/j.poly.2017.03.049> (Impact factor: 3.052).
14. Adsorption properties of graphene towards the ephedrine – A frequently used molecule in sport, S. Armakovic, S.J. Armakovic, B.T. Tomic, **Renjith Raveendran Pillai**, C. Y. Panicker, Computational and Theoretical Chemistry, ISSN: 2210-271X, (2017), 1124, 39,
<https://doi.org/10.1016/j.comptc.2017.12.009> (Impact Factor: 1.926).
15. Novel Synthetic approach, spectroscopic characterization and theoretical studies on global and local reactive properties of a bibenzimidazolyl derivative. K.S. Prasad, N. Nayak, **Renjith Raveendran Pillai**, S. Armakovic, S.J. Armakovic, Journal of Molecular Structure, ISSN: 0022-2860, (2017), 1147, 121,
<https://doi.org/10.1016/j.molstruc.2017.06.073> (Impact Factor: 3.196).
16. Synthesis, Theoretical studies and molecular docking of a novel chlorinated tetracyclic : (Z/E)-3-(1,8-dichloro-9,10-dihydro-9,10-ethanoanthracen-11-yl)acrylaldehyde, M.A. Sultan, A.I. Almansour, **Renjith Raveendran Pillai**, R.S. Kumar, N. Arumugam, S. Armakovic, S.J. Armakovic, S.M. Soliman, Journal of Molecular structure, ISSN: 0022-

- 2860, (2017), 1150, 358, <https://doi.org/10.1016/j.molstruc.2017.08.101> (Impact Factor : 3.196).
17. Synthesis, XRD Crystal structure, Spectroscopic Characterization (FT-IR, ^1H and ^{13}C NMR), DFT studies using molecular dynamics simulations and evaluation of antimicrobial and antioxidant activities of a novel chalcone. D.A. Zainuri, S. Arshad, N.C.Khalib, I.A. Razak, **Renjith Raveendran Pillai**, S.F.Sulaiman, N.S.Hashim, K.L.Ooi, S. Armakovic, S.J.Armakovic, C.Y.Panicker, C.V.Alsenoy, Journal of MolecularStructure,ISSN:0022-2860,(2017),1128,520, <https://doi.org/10.1016/j.molstruc.2016.09.022> (Impact Factor: 3.196).
18. Vibrational spectroscopic investigations, molecular dynamics simulations and molecular docking studies of N'-diphenylmethylidene-5-methyl-1H-pyrazole-3-carbohydrazide. **Renjith Raveendran Pillai**, V.V. Menon, Y.S. Mary, S. Armakovic, S.J. Armakovic, C.Y. Panicker, Journal of molecular structure, ISSN: 0022-2860, (2017), 1130, 208, <https://doi.org/10.1016/j.molstruc.2016.10.032> (Impact Factor: 3.196).
19. Synthesis, Crystal structure, Hirshfeld surface analysis, Spectroscopic characterization, reactivity study by DFT and MD approaches and molecular docking study of a novel chalcone derivative. S.Arshad, **Renjith Raveendran Pillai**, D. A. Zainuri, N.C. Khalib, I.A. Razak, S. Armakovic, S.J. Armakovic, C.Y. Panicker, C.V. Alsenoy, Journal of Molecular structure, ISSN: 0022-2860, (2017), 1135, 234, <https://doi.org/10.1016/j.molstruc.2017.01.080> (Impact Factor: 3.196).
20. Synthesis, XRD crystal structure, spectroscopic characterization, local reactive properties using DFT and molecular dynamics simulations and molecular docking study of (E)-1-(4-bromophenyl)-3-(4-(trifluoromethoxy)phenyl)prop-2-en-1-one, S. Arshad, **Renjith Raveendran Pillai**, D.A. Zainuri, N.C. Khalib, I.A. Razak, S. Armakovic, S.J. Armakovic, R. Renjith, C.Y. Panicker, C.V. Alsenoy, Journal of Molecular structure, ISSN: 0022-2860, (2017), 1137, 419, <https://doi.org/10.1016/j.molstruc.2017.02.045> (Impact Factor: 3.196).
21. Synthesis, Crystal structure analysis, molecular docking studies and density functional theory predictions of the local reactive properties and degradation properties of a novel halochalcone. S. Arshad, **Renjith Raveendran Pillai**, D.A. Zainuri, N.C. Khalib, I.A. Razak, S. Armakovic, S.J. Armakovic, Journal of Molecular structure, ISSN: 0022-2860, (2017), 1144, 246, <https://doi.org/10.1016/j.molstruc.2017.05.052> (Impact Factor: 1.753).

22. Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO-LUMO analysis and molecular docking studies of 1-hydroxy-4,5,8-tris(4-methoxyphenyl)anthraquinone, **R. Renjith**, Y.S. Mary, H.T. Varghese, C.Y. Panicker, T. Thiemann, A. Shereef, A.A. Al-Saadi, Journal of Physics and Chemistry of Solids, ISSN: 0022-3697, (2015), 87, 110, <https://doi.org/10.1016/j.jpcs.2015.07.024> (Impact Factor : 3.995).
23. Spectroscopic (FT-IR, FT-Raman) investigations and quantum chemical calculations of 1,7,8,9-tetrachloro-10,10-dimethoxy-4-{3[4-(3-methoxyphenyl)piperazine-1-yl]propyl}-4-azatricyclo[5.2.1.0^{2,6}]dec-8-ene-3,5-dione. **R. Renjith**, Y.S. Mary, C.Y. Panicker, H.T. Varghese, M.Pakosinska-Parys, C.V. Alsenoy, A.A. Al-Saadi, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, ISSN: 1386-1425, (2014), 129, 438, <https://doi.org/10.1016/j.saa.2014.03.077> (Impact Factor – 4.098).
24. Vibrational spectroscopic and computational study of 1,7,8,9-Tetrachloro-4-(4-bromobutyl)-10,10-dimethoxy-4-aza-tricyclo[5.2.1.0^{2,6}]dec-8-ene-3,5-dione, **R. Renjith**, Y.S. Mary, C.Y. Panicker, H.T. Varghese, M. Pakosinska-Parys, C.V. Alsenoy, T.K. Manojkumar, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, ISSN: 1386-1425, (2014),124, 480, <https://doi.org/10.1016/j.saa.2014.01.040> (Impact Factor: 4.098).
25. Spectroscopic (FT-IR, FT-Raman), first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 1,7,8,9-tetrachloro-10,10-dimethoxy-4[3-(4-phenyl)piperazine-1-yl]propyl]-4-azatricyclo[5.2.1.0^{2,6}]dec-8-ene-3,5-dione by density functional methods, **R. Renjith**, Y.S. Mary, C.Y. Panicker, H.T. Varghese, M. Pakosinska-Parys, C.V. Alsenoy, T.K. Manojkumar, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, ISSN: 1386-1425, (2014), 124, 500, <https://doi.org/10.1016/j.saa.2014.01.045> (Impact Factor : 4.098).
26. Vibrational Spectra, Molecular structure, NBO, HOMO-LUMO and first order hyperpolarizability analysis of 1,4-bis(4-formylphenyl)anthraquinone by density functional theory, **R. Renjith**, Y.S. Mary, H.T. Varghese, C.Y. Panicker, T. Thiemann, C.V. Alsenoy, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, ISSN: 1386-1425, (2014), 131, 225, <https://doi.org/10.1016/j.saa.2014.04.085> (Impact Factor : 4.098).

National Publications

1. Vibrational Spectroscopic Studies of 4-chloro-3-methylphenol, Rajeev T. Ulahannan, R. Renjith, J.B. Bhagyasree, Hema Tresa Varghese, C. Yohannan Panicker, *Oriental Journal of Chemistry*, 2013 (29) 347.
2. FT-IR, FT-Raman and Computational study of Phenylurea, Hema Tresa Varghese, J.B. Bhagyasree, Rajeev T. Ulahannan, R. Renjith, C. Yohannan Panicker, *Oriental Journal of Chemistry*, 2013 (29) 361.
3. FT-IR, FT-Raman and Computational Study of p-Acetylbenzonitrile, J.B. Bhagyasree, Rajeev T. Ulahannan, R. Renjith, Hema Tresa Varghese, C. Yohannan Panicker, *Oriental Journal of Chemistry*, 2013 (29) 291.
4. Vibrational Spectroscopic Study of 3-hydroxyacetophenone, Rajeev T. Ulahannan, R. Renjith, J.B. Bhagyasree, Hema Tresa Varghese, C. Yohannan Panicker, *Ultra Scientist* 2013 (25) 1-8.
5. FT-IR, FT-Raman and Quantum Chemical Calculations of 1-phenylpyrrole, R. Renjith, J.B. Bhagyasree, Rajeev T. Ulahannan, Hema Tresa Varghese, C. Yohannan Panicker, *Oriental Journal of Chemistry*, 29 (2013) 321.
6. Spectroscopic Investigations of methyl trimethylacetate, Rajeev T. Ulahannan, R. Renjith, J.B. Bhagyasree, G. Krishnakumar, Hema Tresa Varghese, C. Yohannan Panicker, *Ultra Scientist*, 2013 (25) 9-16.
7. FT-IR, FT-Raman and quantum chemical calculations of 5-chloromethyl-2-oxazolidinone, R. Renjith, Rajeev T. Ulahannan, J.B. Bhagyasree, Hema Tresa Varghese, C. Yohannan Panicker, *Ultra Scientist*, 2013 (25) 39-46.
8. FT-IR, FT-Raman and quantum chemical calculations of 1,2-cyclohexanediol, R. Renjith, Rajeev T. Ulahannan, J.B. Bhagyasree, Hema Tresa Varghese, C. Yohannan Panicker, *Ultra Scientist*, 2013 (25) 97-103.