Renjith Raveendran Pillai, Ph.D.

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Research Interests

- **Application of Computational Chemistry techniques for predicting material properties**.
- **Structural and dynamic properties of high energetic materials**.
- **Development of functional materials for non-linear optical and optoelectronic applications**.
- **Modeling of 2D- nanomaterials for biosensing applications**.

Research Expertise

Modeling Methods	**DFT, molecular dynamics, molecular docking**.
Program Packages	**Gaussian, Autodock, Multiwfn, VMD etc.**.

Employment History

2023 – · · · · **Assistant Professor**, Department of Physics, Government College Kasaragod, Vidyanagar, KasaragodKerala, India-671121.

2021 – 2023 **Assistant Professor**, Department of Physics, University College, Thiruvananthapuram, Kerala, India-695034.

2019 – 2021 **Assistant Professor of Physics**, Central Polytechnic College, Vattiyoorkavu, Thiruvananthapuram, Kerala, India-695013.

2017 – 2019 **Assistant Professor**, Department of Physics, T.K.M. College of Arts and Science, Karicode, Kollam, Kerala, India-691005.

2016 – 2017 **UGC-FDP Guest Lecturer**, Department of Physics, S.N. College, Varkkala, Shivagiri, Kerala, India-695145.

Education

2011 – 2016 **Ph.D., University of Kerala** Thiruvananthapuram, Kerala, India.
Thesis title: *Spectroscopic Investigations of Certain Azatricyclo and Anthraquinone derivatives.*

2008 – 2010 **M.Sc. Physics**, University of Kerala, Thiruvananthapuram, Kerala, India.

2005 – 2008 **B.Sc. Physics**, University of Kerala, Thiruvananthapuram, Kerala, India.

Publications

Journal Articles

1. Aneesh, K. R., Al-Otaibi, J. S., Mary, Y., Thomas, R., & **Renjith**, **R.** (2024). Solvent effects and raman enhancement during the adsorption of atrazine on pristine ag, au, cu and mixed clusters. *Computational and Theoretical Chemistry*, *1237*, 114628. https://doi.org/https://doi.org/10.1016/j.comptc.2024.114628

2. Aneesh Kumar, R., Jamelah Al-Otaibi, S., Sheena Mary, Y., Shyma Mary, Y., Acharjee, N., Thomas, R., **Renjith**, **R.**, & Leena, T. (2024). Surface adsorption of adenine on pristine and b/n/o/p-doped coronene as a biosensing substrate for dna detection- dft study. *Journal of Molecular Liquids*, *393*, 123546. https://doi.org/https://doi.org/10.1016/j.molliq.2023.123546

3. Dhanya P., K., Chandran R., P., Vijayan Nair, S., & **Renjith**, **R.** (2024). Non-linear optical properties of 2,7-naphthyridine derivatives for optical switching applications: A dft study. *New J. Chem.*, *48*, 2689–2706. https://doi.org/10.1039/D3NJ04885C

4. Dhanya P., K., **Renjith**, **R.**, Al-Otaibi, J. S., & Mary, Y. S. (2024). Dft insights into the nonlinear optical properties of azulene-stilbene dyads for photonics and optoelectronics. *Journal of Molecular Liquids*, *414*, 126053. https://doi.org/https://doi.org/10.1016/j.molliq.2024.126053

5. Archana, V. P., Armaković, S. J., Armaković, S., Celik, I., Bhagyasree, J., Dinesh Babu, K., Rudrapal, M., Divya, I. S., & **Renjith**, **R.** (2023). Exploring the stuctural, photophysical and optoelectronic properties of a diaryl heptanoid curcum derivative and identification as a sars-cov-2 inhibitor. *Journal of Molecular Structure*, *1281*, 135110. https://doi.org/10.1016/j.molstruc.2023.135110

6. Çevik, U. A., Celik, I., Işık, A., **Renjith**, **R.**, Tallei, T. E., Yadav, R., Özkay, Y., & Kaplancıklı, Z. A. (2022). Synthesis, molecular modeling, quantum mechanical calculations and adme estimation studies of benzimidazole-oxadiazole derivatives as potent antifungal agents. *Journal of Molecular Structure*, *1252*, 132095. https://doi.org/https://doi.org/10.1016/j.molstruc.2021.132095

7. Karrouchi, K., Celik, I., Fettach, S., Karthick, T., Bougrin, K., Radi, S., Faouzi, M. E. A., Ansar, M., & **Renjith**, **R.** (2022a). Synthesis and investigations of reactive properties, photophysical properties and biological activities of a pyrazole-triazole hybrid molecule. *Journal of Molecular Structure*, *1265*, 133363. https://doi.org/10.1016/j.molstruc.2022.133363

8. Karrouchi, K., Celik, I., Fettach, S., Karthick, T., Bougrin, K., Radi, S., Faouzi, M. E. A., Ansar, M., & **Renjith**, **R.** (2022b). Synthesis, molecular modeling, quantum mechanical calculations and adme estimation studies of benzimidazole-oxadiazole derivatives as potent antifungal agents. *Journal of Molecular Structure*, *1252*, 132095. https://doi.org/10.1016/j.molstruc.2021.132095

9. Poojith, N., Kigga, M., John Rose, J., Potla, K. M., Vankayalapati, S., Chinnam, S., Adimoole, S. P., & **Renjith**, **R.** (2022). Structural, spectroscopic, and in silico studies of 3-(dimethylamino)-1-(thiophen-2-yl)propan-1-ol: A potential antidepressant agent. *Journal of Molecular Structure*, *1250*, 131859. https://doi.org/10.1016/j.molstruc.2021.131859

10. Poojith, N., Rani, N. U., Potla, K. M., John Rose, J., Suchetan, P., **Renjith**, **R.**, & Vankayalapati, S. (2021). An analysis of structural, spectroscopic, quantum chemical and in silico studies of ethyl 3-[(pyridin-2-yl)amino]propanoate: A potential thrombin inhibitor. *Journal of Molecular Structure*, *1226*, 129378. https://doi.org/10.1016/j.molstruc.2020.129378

11. Shetgaonkar, S. E., Kollur, S. P., **Renjith**, **R.**, Thangavel, K., Armaković, S. J., Armaković, S., Shivamallu, C., Amachawadi, R. G., Syed, A., Elgorban, A. M., Bahkali, A. H., & Singh, F. V. (2021). Investigation of pharmaceutical importance of 2h-pyran-2-one analogues via computational approaches. *Symmetry*, *13*(9), 1619. https://doi.org/10.3390/sym13091619

12. Sultan, M., Ghabbour, H., Soliman, S., **Renjith**, **R.**, & Mansour, S. G. (2021). Synthesis, hirshfeld surface analysis and dft studies of ethano-tetracyclic tetracine derivatives. *Journal of Chemical Crystallography*, *51*, 196–204. https://doi.org/10.1007/s10870-020-00841-6

13 Prasad, K. S., **Renjith**, **R.**, Ghimire, M. P., Ray, R., Richter, M., Shivamallu, C., Jain, A. S., Prasad, S. K., P, S., Armaković, S., Armaković, S. J., & Amachawadi, R. G. (2020). 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. *Journal of Molecular Structure*, *1217*, 128445. https://doi.org/10.1016/j.molstruc.2020.128445

14 Prasad, K. S., **Renjith**, **R.**, Shivamallu, C., Prasad, S. K., Jain, A. S., Pradeep, S., Armaković, S., Armaković, S. J., Srinivasa, C., Kallimani, S., Amachawadi, R. G., Ankegowda, V. M., Marraiki, N., Elgorban, A. M., & Syed, A. (2020). Tumoricidal potential of novel amino-1,10-phenanthroline derived imine ligands: Chemical preparation, structure, and biological investigations. *Molecules*, *25*(12), 2865. https://doi.org/10.3390/molecules25122865

15 Prasad, K. S., **Renjith**, **R.**, Armaković, S., & Armaković, S. J. (2019). Photophysical properties and theoretical investigations of newly synthesized pyrene-naphthalene based schiff base ligand and its copper(ii) complexes. *Inorganica Chimica Acta*, *486*, 698–703. https://doi.org/10.1016/j.ica.2018.11.045

16 **Renjith**, **R.**, Karrouchi, K., Fettach, S., Armaković, S., Armaković, S. J., Brik, Y., Taoufik, J., Radi, S., El Abbes Faouzi, M., & Ansar, M. (2019). Synthesis, spectroscopic characterization, reactive properties by dft calculations, molecular dynamics simulations and biological evaluation of schiff bases tethered 1,2,4-triazole and pyrazole rings. *Journal of Molecular Structure*, *1177*, 47–54. https://doi.org/10.1016/j.molstruc.2018.09.037

17 Armaković, S., Armaković, S. J., Tomić, B. T., **Renjith**, **R.**, & Panicker, C. Y. (2018). Adsorption properties of graphene towards the ephedrine – a frequently used molecule in sport. *Computational and Theoretical Chemistry*, *1124*, 39–50. https://doi.org/10.1016/j.comptc.2017.12.009

18 Nayak, N., Prasad, K. S., **Renjith**, **R.**, Armaković, S., & Armaković, S. J. (2018). Remarkable colorimetric sensing behavior of pyrazole-based chemosensor towards cu(ii) ion detection: Synthesis, characterization and theoretical investigations. *RSC Adv.*, *8*, 18023–18029. https://doi.org/10.1039/C8RA02905A

19 Arshad, S., **Renjith**, **R.**, Zainuri, D. A., Khalib, N. C., Razak, I. A., Armaković, S., & Armaković, S. J. (2017). Synthesis, crystal structure analysis, molecular docking studies and density functional theory predictions of the local reactive properties and degradation properties of a novel halochalcone. *Journal of Molecular Structure*, *1144*, 246–253. https://doi.org/10.1016/j.molstruc.2017.05.052

20 Arshad, S., **Renjith**, **R.**, Zainuri, D. A., Khalib, N. C., Razak, I. A., Armaković, S., Armaković, S. J., Panicker, C. Y., & Van Alsenoy, C. (2017). Synthesis, crystal structure, hirshfeld surface analysis, spectroscopic characterization, reactivity study by dft and md approaches and molecular docking study of a novel chalcone derivative. *Journal of Molecular Structure*, *1135*, 234–246. https://doi.org/10.1016/j.molstruc.2017.01.080

21 Arshad, S., **Renjith**, **R.**, Zainuri, D. A., Khalib, N. C., Razak, I. A., Armaković, S., Armaković, S. J., Renjith, R., Panicker, C. Y., & Van Alsenoy, C. (2017). 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. *Journal of Molecular Structure*, *1137*, 419–430. https://doi.org/10.1016/j.molstruc.2017.02.045

22 Prasad, K. S., Nayak, N., **Renjith**, **R.**, Armaković, S., & Armaković, S. J. (2017). Novel synthetic approach, spectroscopic characterization and theoretical studies on global and local reactive properties of a bibenzimidazolyl derivative. *Journal of Molecular Structure*, *1147*, 121–128. https://doi.org/10.1016/j.molstruc.2017.06.073

23 **Renjith**, **R.**, Menon, V. V., Mary, Y. S., Armaković, S., Armaković, S. J., & Panicker, C. Y. (2017). Vibrational spectroscopic investigations, molecular dynamic simulations and molecular docking studies of n-diphenylmethylidene-5-methyl-1h-pyrazole-3-carbohydrazide. *Journal of Molecular Structure*, *1130*, 208–222. https://doi.org/10.1016/j.molstruc.2016.10.032

24 Shiva Prasad, K., **Renjith**, **R.**, Armaković, S., & Armaković, S. J. (2017). 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. *Polyhedron*, *129*, 141–148. https://doi.org/10.1016/j.poly.2017.03.049

25 Sultan, M. A., Almansour, A. I., **Renjith**, **R.**, Kumar, R. S., Arumugam, N., Armaković, S., Armaković, S. J., & Soliman, S. M. (2017). 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. *Journal of Molecular Structure*, *1150*, 358–365. https://doi.org/10.1016/j.molstruc.2017.08.101

26 Zainuri, D. A., Arshad, S., Khalib, N. C., Razak, I. A., **Renjith**, **R.**, Sulaiman, S. F., Hashim, N. S., Ooi, K. L., Armaković, S., Armaković, S. J., Panicker, C. Y., & Van Alsenoy, C. (2017). Synthesis, xrd crystal structure, spectroscopic characterization (ft-ir, 1h and 13c nmr), dft studies, chemical reactivity and bond dissociation energy studies using molecular dynamics simulations and evaluation of antimicrobial and antioxidant activities of a novel chalcone derivative, (e)-1-(4-bromophenyl)-3-(4-iodophenyl)prop-2-en-1-one. *Journal of Molecular Structure*, *1128*, 520–533. https://doi.org/10.1016/j.molstruc.2016.09.022

27 **Renjith**, **R.**, Sheena Mary, Y., Tresa Varghese, H., Yohannan Panicker, C., Thiemann, T., Shereef, A., & Al-Saadi, A. A. (2015). Spectroscopic investigation (ft-ir and ft-raman), vibrational assignments, homo–lumo analysis and molecular docking study of 1-hydroxy-4,5,8-tris(4-methoxyphenyl) anthraquinone. *Journal of Physics and Chemistry of Solids*, *87*, 110–121. https://doi.org/10.1016/j.jpcs.2015.07.024

28 **Renjith**, **R.**, Mary, Y. S., Panicker, C. Y., Varghese, H. T., Pakosińska-Parys, M., Alsenoy, C., & Manojkumar, T. (2014). Vibrational spectroscopic and computational study of 1,7,8,9-tetrachloro-4-(4-bromo-butyl)-10,10-dimethoxy-4-aza-tricyclo[5.2.1.02,6] dec-8-ene-3,5-dione. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, *124*, 480–491. https://doi.org/10.1016/j.saa.2014.01.040

29 **Renjith**, **R.**, Mary, Y. S., Panicker, C. Y., Varghese, H. T., Pakosińska-Parys, M., Van Alsenoy, C., & Al-Saadi, A. A. (2014). Spectroscopic (ft-ir, ft-raman) investigations and quantum chemical calculations of 1,7,8,9-tetrachloro-10,10-dimethoxy-4-3-[4-(3-methoxyphenyl)piperazin-1-yl]propyl-4-azatricyclo[5.2.1.02,6]dec-8-ene-3,5-dione. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, *129*, 438–450. https://doi.org/10.1016/j.saa.2014.03.077

30 **Renjith**, **R.**, Mary, Y. S., Panicker, C. Y., Varghese, H. T., Pakosińska-Parys, M., Van Alsenoy, C., & Manojkumar, T. (2014). 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-phenylpiperazin-1-yl)propyl]-4-azatricyclo[5.2.1.02,6]dec-8-ene-3,5-dione by density functional methods. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, *124*, 500–513. https://doi.org/10.1016/j.saa.2014.01.045

31 **Renjith**, **R.**, Mary, Y. S., Varghese, H. T., Panicker, C. Y., Thiemann, T., & Van Alsenoy, C. (2014). Vibrational spectra, molecular structure, nbo, homo–lumo and first order hyperpoalarizability analysis of 1,4-bis(4-formylphenyl)anthraquinone by density functional theory. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, *131*, 225–234. https://doi.org/10.1016/j.saa.2014.04.085

Conferences

2023 **Resource Person**- International Seminar on '**Physics of the Future**' organized by Department of Physics, BJM Government College, Chavara, Kollam, Kerala, India.

Paper Presentation- National Seminar on '**Recent Trends in Physics**' organized by Department of Physics, Government College, Kariavattom, Kerala, India.

2021 **Paper Presentation**- International Conference on '**Engrossing Trends in Chemistry**' organized by Department of Polymer Chemistry, Government College, Attingal, Kerala, India.

Research Supervision

PhD — Ongoing - 4
Completed - Nil

M.Sc. Project — Completed - 22

Citations in Google Scholar

Total Citations — **502.**
h-index — **14**
i-10 index — **16**

Funded Projects

Ongoing

2023- **Developing Novel Organic π-conjugated Materials using Through Space Charge Transfer Mechanism for NLO Applications**
Funding Agency-**SERB, India**
Amount - **20,89,560 INR**

Awards and Achievements

Awards

2014 **CSIR-UGC SRF**

2011 **GATE**, All India Rank-426.

CSIR-UGC JRF, All India Rank-126.

Organisational Performance

2019 **District Coordinator**, Sasthrapadham-2019, Samagra Shiksha, Kerala, India.

District Coordinator, Sasthrajalakam-2019, SIET, Kerala, India.

Judge, State Science Fair, Kerala, India.

Academic Workshops/Trainings

2023 **Refresher Course in Material Science**, HRDC, University of Kerala, Thiruvananthapuram, India.

2021 **Short Term Course in Materials Characterization Techniques**, Department of MEMS, IIT Indore.

2020 **Refresher Course in Material Science**, HRDC, University of Kerala, Thiruvananthapuram, India.

Induction Programme for College Teachers, CoESME, IISER PUNE, India

2013 **Science Academies Refresher Course in Quantum Mechanics**, JSS campus, Suttur, Maharashtra, India.

References

Dr. Stevan Armakovic (Collaborator)
Assistant Professor
Faculty of Sciences, Department of Physics
University of Novi Sad, Serbia
stevan.armakovic@df.uns.ac.rs

Dr. Khalid Karrouchi (Collaborator)
Professor
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Dr. Jijo P. Ulahannan (Department Head)
Associate Professor
Department of Physics
Government College, Kasaragod, Kerala, India
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Dr. C. Yohannan Panicker (PhD Advisor, India)
Former Associate Professor
Department of Physics
T.K.M. College of Arts and Science, Kerala, India
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