

# Renjith Raveendran Pillai, Ph.D.

✉ renjithkadavoor@gmail.com; drrenjith@gck.ac.in

☎ +918281560152

🌐 <https://orcid.org/0000-0002-0669-4045>

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



## 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, Kerala, 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, Kari-code, 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 Kumar, R., Al-Otaibi, J. S., Mary, Y. S., Mary, Y. S., Acharjee, N., Thomas, R., & **Renjith, R.** (2023). Surface adsorption of adenine on pristine and doped (b, n, o and p) coronene nanosheets as a biosensing substrate for dna detection- dft study. *Journal of Molecular Liquids*, Accepted for Publication.
- 2 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 structural, photophysical and optoelectronic properties of a diaryl heptanoid curcumin derivative and identification as a sars-cov-2 inhibitor. *Journal of Molecular Structure*, 1281, 135110. <https://doi.org/10.1016/j.molstruc.2023.135110>
- 3 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>
- 4 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>
- 5 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>
- 6 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>
- 7 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>
- 8 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>
- 9 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>
- 10 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>
- 11 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>



- 12 **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>
- 13 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>
- 14 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>
- 15 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>
- 16 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>
- 17 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>
- 18 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>
- 19 **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-diphenylmethylened-5-methyl-1h-pyrazole-3-carbohydrazide. *Journal of Molecular Structure*, *1130*, 208–222. <https://doi.org/10.1016/j.molstruc.2016.10.032>
- 20 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>
- 21 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>
- 22 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>

- 23 **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>
- 24 **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[5.2.1.0<sub>2,6</sub>] 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>
- 25 **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[5.2.1.0<sub>2,6</sub>]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>
- 26 **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[5.2.1.0<sub>2,6</sub>]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>
- 27 **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 hyperpolarizability 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  **Paper Presentation**, National Seminar on 'Recent Trends in Physics'.
- 2021  **Paper Presentation**, International Conference on 'Engrossing Trends in Chemistry'.

## Research Supervision

- PhD  Ongoing - 4  
Completed - Nil
- M.Sc. Project  Completed - 22


## Citations in Google Scholar

- Total Citations  428.
- h-index  13
- i-10 index  15

## Funded Projects

---




### Ongoing

- 2023-  **Developing Novel Organic  $\pi$ -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.armacovic@df.uns.ac.rs](mailto:stevan.armacovic@df.uns.ac.rs)

**Dr. Jijo P. Ulahannan (Department Head)**

Associate Professor

Department of Physics

Government College, Kasaragod, Kerala, India

✉ [jijo\(at\)gck.ac.in](mailto:jijo(at)gck.ac.in)

**Dr. Khalid Karrouchi (Collaborator)**

Professor

Faculty of Medicine and Pharmacy

Laboratory of Medicinal Chemistry

University Mohammed V in Rabat, Morocco

✉ [khalid.karrouchi@um5s.net.ma](mailto:khalid.karrouchi@um5s.net.ma)

**Dr. C. Yohannan Panicker (PhD Advisor, India)**

Former Associate Professor

Department of Physics

T.K.M. College of Arts and Science, Kerala, India

✉ [cyphyp@gmail.com](mailto:cyphyp@gmail.com)