

# RAHUL SURESH

Postdoctoral researcher trained in physics and biology, with strong communication skills developed from extensive research experience and ability to work independently or as part of a team. Special expertise in the following areas:

- Density functional theory calculations
- Molecular dynamics simulations
- Experimental synthesis of Nano materials (Graphene, ZnO and CdS)
- Programming

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## Education

Coimbatore  
July 2020

**Bharathiar University**  
Ph.D. (Molecular Quantum Physics)  
DST-PURSE fellowship award for 2017-2018  
and 2018-2019

Coimbatore  
May 2015

**PSG College of Arts and Science**  
M.Sc. (Physics), CGPA – 7.2

Coimbatore  
May 2013

**PSG College of Arts and Science**  
B.Sc. (Physics), CGPA – 6.6



## Leadership Experience

Coimbatore  
Feb 2021

**Shrishakthi Institute of Engineering and Technology**  
Assistant professor, Department of Physics

Coimbatore  
July 2017

**Bharathiar University**  
Organized discussion group (15+ members) focused  
on current events in Molecular Quantum Physics

Coimbatore  
June 2017 –  
Dec 2018

**Private tutor**  
Tutored 35 students in Coimbatore in Math and  
Science

Coimbatore  
June – Dec  
2018

**Teaching Fellow** *Molecular quantum physics*  
Presented 3 lectures during semester

Coimbatore  
2014

Volunteered in organizing SAHAYAM'14, A cultural  
and literary event for differently abled children



## Technical skills

**Software: Gaussian, VASP, Siesta,  
Gromacs, CHARMM, NAMD**

**Hands-on experience in MATLAB  
and Python**



## Soft skills

**Communicator**

**Critical Thinking**

**Analytical**

**Decision Maker**

## Languages

**Malayalam**

**English**

**Tamil**

**French**



## Postdoctoral Research

### Siberian federal University

- Senior research fellow at International research center of spectroscopy and quantum chemistry, Krasnoyarsk, Russia.

Currently, working on

- ❖ Exfoliation of 2D materials from layered and non-layered bulk materials and identify the potential material with magnetic properties for quantum applications.
- ❖ Identification of NFE bands in fullerene material and hence to reduce the bandgap using endohedral doping.
- ❖ Charged defects calculation in Ferrite derivatives.
- ❖ Study of the mechanism in the formation of C18 polymer from their precursor salts.



## Research Experience

### Bharathiar University

- Synthesis and fabrication of graphene and CdS based nanomaterial for the detection of radio nuclei.
- Identification of activation mechanism pathway of adrenoceptors involved in sympathetic nervous system signaling using simulation methods.
- Establishing porphyrin as an adsorbing material for toxic gases using density functional theory.
- Designing of 2-D porphyrin covalent organic frameworks as an electrode for the application of batteries.
- Application of 2-D sheet of porphyrin as an active material in the adsorption of greenhouse gases and dyes.
- Electronic and transport properties of 1-D nanotubes of porphyrin.
- Molecular dynamic simulation of heterodimerization of CRHR and Vasopressin receptor proteins.
- Development of 1D organic nanotube as an active electrode for solid-state applications.

### IIIT-Hyderabad

- Intern at IIIT-Hyderabad on parameterization of small molecules and heterodimerization of GPCR proteins – A MD based prediction method

### Non-Destructive Testing (2013-2016)

- Certified for NDT Level II Magnetic Particle Testing from SQS institute of NDT



## Publications

1. Magnetite nanoparticles decorated reduced graphene oxide composite as an efficient and recoverable adsorbent for the removal of caesium and strontium ions; *Ind. Eng. Chem. Res.* **2018**, *57*, **4**, 1225–1232.
2. Ab initio studies of adsorption of Haloarenes on Heme group; *J Mol Model* **26**, **6** (2020).
3. Molecular dynamics simulation involved in expounding the activation of adrenoceptors by sympathetic nervous system signaling; Structural Chemistry; *Struct Chem* (2020). [10.1007/s11224-020-01553-5](https://doi.org/10.1007/s11224-020-01553-5)
4. Quantum chemical support on the 2-Dimensional assembly of porphyrin rings in the application of Energy Storage Devices; Journal of Physical Chemistry C; *J. Phys. Chem. C* **2020**, *124*, **18**, 9712–9723
5. Adsorption of greenhouse gases on the surface of covalent organic framework of porphyrin – An ab initio study (Physica E: Low-dimensional systems and nanostructures – *Phys. E Low-Dimensional Syst. Nanostructures.* **126** (2021) 114448. [10.1016/j.physe.2020.114448](https://doi.org/10.1016/j.physe.2020.114448).
6. A first principle study of adsorption of Haloalkenes on Heme molecule; [10.1007/s00894-021-04821-1](https://doi.org/10.1007/s00894-021-04821-1).
7. Nanotechnology-based solution to combat zoonotic viruses with special attention to SARS, MERS and COVID19: Detection protection and medication, Microbial pathogenesis; [10.1016/j.micpath.2021.105133](https://doi.org/10.1016/j.micpath.2021.105133).
8. Amine terminated polyynes as candidates for molecular wire; [10.1016/j.physe.2021.115045](https://doi.org/10.1016/j.physe.2021.115045).
9. Adsorptive removal of noxious Atrazine using Graphene oxide nanosheets: Insights to process optimization, equilibrium, kinetics, and density functional theory calculations; [10.1016/j.envres.2021.111428](https://doi.org/10.1016/j.envres.2021.111428)
10. Adsorption of Volatile Organic Compounds on Pristine and Defected Nanographene; [10.1016/j.comptc.2022.113664](https://doi.org/10.1016/j.comptc.2022.113664)
11. Evolution of Li@C60 superatom molecular orbitals on Cu(111) surface. (Communicated in Acta Materialia)
12. EnsemblQS: A stacked ensemble learning framework for sequence based prediction of quorum sensing peptides (Communicated in Journal of Microbiology)
13. Santalol isomers prevent transthyretin amyloidogenesis and associated pathologies in *Caenorhabditis elegans* by activating SKN-1/Nrf2, autophagy, and proteasome (Communicated in ACS Chemical Neuroscience)
14. Electronic and optical properties of sulfur and selenosulfur – Ab initio calculations (Communicated to PCCP)
15. Adsorption Studies of Dye Molecule on Two-dimensional Assembly of Porphyrin using Density Functional Theory for the Application of Dye Sensitized Solar Cells (Communicated to chemistry letters).
16. Machine learning assisted screening of peptide ligands targeting human voltage gated potassium channel KV1.3 and its molecular dynamics simulation (Yet to communicate)
17. Enzymatic degradation of piroxicam reduces toxicity in the Zebrafish model (Yet to communicate).

## Conference/Workshop

### **BITS Pilani**

- Presented poster at Theoretical chemistry symposium 2019

### **National Centre for Cell Science**

- Presented poster at 10th annual meeting of Proteomics society India 2018
- Participated in workshop by APTECH on "Network Essential"

### **Bharathiar University**

- Attended the SERC school on nuclear physics 2017
- Participated in National seminar on "Advanced Functional Materials" organized by Department of Physics
- Attended the symposium on Materials and Research Techniques organized by Department of Physics and Medical Physics
- Presented a paper in National Symposium on Science of Nano held at Bharathiar University

### **PSG College of Technology**

- Participated in the International workshop on Theoretical and Experimental Physics organized by PSG College of Technology
- Attended a National workshop on Advanced Materials organized by GRD Centre for Materials Research, PSG College of Technology

### **PSGR Krishnammal College for Women**

- Participated in Lecture workshop on Applications of LASER Technology in Science, Research and Innovation conducted at PSGR Krishnammal College for Women

### **BioDiscovery Group, Bengaluru**

- Attended 2 days Workshop on Molecular Modelling & Dynamics 2016

## Current Project

- Electronic and spin transport properties of 1-dimensional organic nanotube for spintronic applications
- Estimating the properties of organic nanotubes in the application of energy storage devices using Lammmps and Siesta.
- Modelling of vasopressin receptor proteins using ML based modelling techniques.
- High-throughput calculation in identifying exfoliable 2-dimensional material from non-layered bulk material.

## References

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## Personal Details

**Father's name** : **Late. Mr. V.B. Suresh Babu**

**Date of Birth** : **04 Feb 1993**

**Gender** : **Male**

**Nationality** : **Indian**