

# Prajval K

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## EDUCATION

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**Indian Institute of Science and Education Research, Thiruvananthapuram** Aug. 2022 – Present  
*2nd Year, Integrated BS-MS* *Current CGPA: 9.05/10*

**Courses:** Quantum Chemistry, General Chemistry, Real Analysis, Linear Algebra, Spectroscopy, Mechanics, Electrodynamics, Biochemistry, Scientific and Numeric Computation

**Self-Learnt Topics:** Numerical Analysis in ODEs, Introductory Fluid Dynamics, Data Structure and Algorithms

**Fellowship:** DST-INSPIRE SHE Scholar (2022-Present)

**Swamy Vivekananda Rural Pre-University College (SVRPUC)** May 2020 – June 2022  
*Karnataka State Board* *96%*

**Nazareth School, Bangalore** Apr. 2010 – May 2020  
*Grade 1-10, CICSE Board* *96%*

## INTERNSHIPS AND WORKSHOPS

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**Noble Gas Dimers** | IISER TVM Feb. 2023 – Present  
Involved in a computational modelling internship about studying noble gas dimer interaction under the supervision of Prof. R S Swathi (IISER TVM) and her research group.

**High Performance Computing in Bioinformatics** | Workshop Organized by IIT Kharagpur  
Attended a workshop organized at IIT Kharagpur under the aegis of National Supercomputing Mission (NSM), focused on molecular dynamics, protein folding and design, protein docking, with hands-on training on GROMACS and Autodock Vina.

**High Performance Computing in Complex and Moving Geometries** | Workshop Organized by IIT Kharagpur  
Attended a workshop organized by IIT Kharagpur at Jadavpur University, Kolkata under the aegis of National Supercomputing Mission (NSM), with hands-on training on large-scale computational techniques for compressible and incompressible fluid flow using openFOAM.

## RESEARCH PROJECTS

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**Advancements in Theoretical Chemistry Presentation** | Reading Project Feb. 2023 – Apr. 2023

- Reading about the academic research of frontier people in the field of Theoretical Chemistry to understand the scope of the subject. This included the works of older scientists, such as Pauling, Mulliken, Onsager, Prigogine, Fukui-Hoffmann, Lee-Herschbach-Polanyi, and Marcus, as well as recent well-recognized results, such as the conception and development of Density Functional Theory (DFT) by Kohn-Pople and multiscale modelling approaches of Karplus-Levitt-Warshell.
- This was presented to the research group of Prof. R S Swathi in Apr. 2023.

**Study of Noble Gas Dimers** | Project under Prof. R S Swathi, IISER TVM Apr. 2023 – Present

- Developed a program in Python for analysis into Lennard-Jones (LJ) and Improved Lennard-Jones (ILJ) schemes for noble gas dimer molecules.
- Worked with Gauss-Newton and Simplex algorithms in Python for curve-fitting and non-linear root finding.
- We are also looking into noble gas dimer-dimer interactions and multi-dimensional configurations and are also interested in developing a parallelized approach to minimizing configuration energies.

**Water Rocket Analysis** | Orbiton Labs, Independent Student Group Study March. 2023 – Present

- Developed a simulation program in C++ (GitHub: [@orbitonlabs/fastsim](https://github.com/orbitonlabs/fastsim)) for the design and analysis of a simple model of water rockets.
- For academic completeness, the program includes a from-scratch implementation of simpler Euler ODE solvers and more complex Runge-Kutta (RK) methods, including implicit and Diagonally Implicit RK methods using a custom linear algebra system.

- Our student research group is interested in finding physical or statistical models that resemble experimental and fluid dynamics results for water rockets at high-pressure limits. We have presented our results in Anvesha 2023, our flagship annual student exhibition.
- Additionally, we are also looking into developing a novel propulsion system based on Liquid Nitrogen water rocket engines and low-latency flight correction in the future. We are also working on a parallelized version of the simulation using openMPI and openACC libraries.

## RESEARCH INTERESTS

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I have a keen interest in the computational modelling of physical systems. I am also interested in the numerical study of systems of ODEs, which was a motivating factor towards self-learning numerical methods. I am also intrigued by the theory of Quantum Chemistry and am especially interested in the numerical modelling of chemical systems using a quantum mechanical approach. I am always eager to explore newer waters in computational sciences.

## SKILLS

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**Languages Spoken:** English, Kannada, Hindi, Telugu

**Programming Languages:** C++, Python, Java, HTML/CSS,  $\text{\LaTeX}$

**Programming Tools:** Git/GitHub, Bash, Matlab, openFOAM

## VOLUNTEERING

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<b>Frontier Symposium in Mathematics 2023</b>   Core Organizer	Feb. 2023
<b>International Genetic Engineering Machine (iGEM) 2023, IISER TVM</b>   Wiki Team Volunteer	Sept. 2023
<b>Inter-IISER Sports Meet 2023</b>   Website Team	Dec. 2023
<b>TEDxIISERTVM 2024</b>   Tech Team	Nov. 2023 – Present
<b>Club Mathematics of IISER TVM (CMIT)</b>   Club Coordinator	Feb. 2023 – Present
<b>Chemical Society of IISER TVM (CSIT)</b>   Club Coordinator	Aug. 2023 – Present
<b>Physics Society of IISER TVM (PSI(T))</b>   Website Volunteer	Oct. 2023 – Present
<b>Ether Magazine</b>   Website Volunteer	Apr. 2023 – Present
<b>Orbiton Labs : Student Rocket Research Group</b>   Team Lead, Numeric Computation	Feb. 2023 – Present
<b>openAOD : Open Source Developer Group</b>   Core Contributor	Jan. 2021 – Jan. 2023