

I am Komma Gnana Spoorthy, a final-year undergraduate student of the Department of Chemistry, enrolled in its five-year integrated Master's degree at the Indian Institute of Technology, Kharagpur.

Since my early secondary education, I have had a keen interest and inclination towards science, and it changed the way I perceive the world. My curiosity drove me to pursue studies in science, and it increased my interest in research. Research allows one to pursue one's interests, to learn something new, hone problem-solving skills, and challenge oneself in new ways. To achieve this, I have been working hard to increase my knowledge and understanding

As a student of India's premier institute, I have been given the right platform to build knowledge in great depth in the field of Chemistry. I have had courses like Introduction to Quantum Chemistry & Spectroscopy, Computational Chemistry, which includes concepts like Metropolis Monte Carlo method, Molecular dynamics, Verlet algorithm, Hartree-Fock method, Density Functional Theory and also Computational Chemistry Laboratory, Group Theory for Chemist and Physics-II contains the basis of quantum chemistry and solid-state and we have a course solid-state chemistry which will further increase my concepts, and these all courses have equipped me with the knowledge and tools to understand Quantum chemistry and computational chemistry in detail. To further enhance my knowledge I took elective courses on Computational Structural Biology and learned concepts like docking and some basics on molecular dynamics simulation and basics of using software like NAMD, Quantum methods in molecular simulations, and Light-induced phenomena in Materials where I have learned concepts like Material spin crossover, Jahn-Teller effect, molecular photonics which still more increased my understanding and interest in the field. I also took up courses like Programming and Data structures, Design & Analysis of Algorithms, Algorithms Laboratory, Machine Learning, High-Performance Parallel Programming which strengthened my programming and computational skills.

Beyond my college courses, I attended Summer research internship at the University of Hyderabad, where I worked on 'Elucidation of structure and reactivity of chemical systems using computational chemistry.' In which I used Gaussian 09 software to do the geometry optimization, estimated the transition state for chemical reactions and equilibrium reactions, and also calculated their rate constants and equilibrium constants and also predicted the minimum energy path of a reaction. I have also applied Multi-configuration time-dependent Hartree (mctdh) calculations on molecules like NOCl, pyrazine.

As a part of my Master's project, I worked on Global optimization using algorithms for which I learned different optimization techniques like Particle swarm optimization, Firefly algorithm, Genetic algorithm, Simulated annealing and implemented new bonobo algorithm on the carbon clusters to find the global minimum structure using bonobo algorithm in python and interfacing with Gaussian software to get the energy values

All these courses and works increased my curiosity and interest to learn more in the field of computational chemistry. It will be exciting and challenging to increase my computational chemistry knowledge by doing research under the prestigious project in IITKGP-University of Manchester Dual Doctoral Degree program for a project under computational Chemistry and helps me giving world-class exposure and also learning important life skills.