STATEMENT OF PURPOSE

The advent of Quantum Mechanics revolutionized the very outlook of man towards nature. The subject of Chemistry also took a new shape. The quest to look inside a molecule or an atom, to look into its structure led to the developments of various theories. It was found that the single body problems were exactly solvable but, various problems aroused in solving many body problems. For solving the many body problems, many theories evolved right from the Hartree-Fock method to the post Hartree-Fock methods like CI, Moller- Plesset perturbation theory, the Coupled Cluster techniques and lastly, the density functional based method DFT. My interest to know the world from the very fundamentals together with the highly intriguing complexities associated with the many-body problems incited in me the interest to take up this field of Quantum Chemistry for my doctoral studies.

Since my Undergraduate days, I felt inclined towards Quantum Chemistry. Exploring the properties of the chemical systems from the very fundamentals always seemed fascinating. That interest led me to join Prof. Pratim Kumar Chattaraj's Theoretical and Computational Chemistry lab at the Department of Chemistry, IIT Kharagpur as an MSc project student. My project is mainly focused on understanding the phenomenon of quantum localization and tunneling in asymmetric double well potentials. I have also done comparative studies between systems to understand the effect of the barrier heights and the strength of the perturbations on the prospect of delocalization (tunneling / over- barrier transitions). I have used Quantum Theory of Motion as the theory to understand the non- classical phenomenon of tunneling. This Project helped me to learn a lot of things regarding Quantum Theory of Motion and Computational Chemistry in general. Another thing to mention, as part of the coursework, I did a project on the benchmark studies for a particular tautomeric reaction where we did the study using 22 different theoretical methods. We have done the calculations using Orca. This project entailed me to understand the electronic structure calculation techniques deeply and also helped me in concretizing my future research plans.

My primary research interest is in Theoretical and Computational Chemistry. During my doctoral studies, I would mainly like to focus on the Electronic structure calculations of various

complicated systems. I would prefer to work on the negative molecular ions using both the DFT and wave function based methods. I would also like to work in the field of Quantum Theory of Motion to look for further insights on the phenomenon of tunneling by modelling real systems. I also feel interested to work on the field of nuclear dynamics in the non-adiabatic regime to study and understand excited state dynamics of molecular systems.

Thus, this joint doctoral program will give me proper exposures and help in shaping my research goals.The auspicious supervisions of Prof. Pratim Kumar Chattaraj and Prof. Paul Popelier, will undoubtedly heighten my understanding on the subject and with the outstanding research facilities of both the institutions, I will get the opportunity to dig deeper into the research and bring out something fruitful for the society.

Yours sincerely,

Bhrigu Chakraborty