Acknowledgements

This is indeed the right place to convey my sincere and heartfelt gratitude to my Ph.D. supervisor Dr. Sourav Pal. I am indebted to him for his constant implicit appreciations, personal considerations and invaluable guidance during the course of this research work. The atmosphere of academic freedom provided by him and his excellent teaching abilities of electronic structure theory were most helpful for me to explore some important aspects of quantum chemistry in my own way. It is my pleasure to keep on records the deep respect and appreciation I have towards him.

It is probably the best time to express my obligations toward my Mathematics and Physics teacher of XII\textsuperscript{th} class, Er. S. K. Agrawal sir, for his world class teaching during my preparation for IIT-JEE. Most of the times in my Ph.D., I had a strong feeling that I was simply following the fundamental concepts of Calculus, Probability and Classical Mechanics, learned from him during those days, to solve my problems related to this thesis work.

I am grateful to Dr. Nayana Vaval for taking my classes at very initial stage of my Ph.D.. She helped me to debug my codes and to correct my papers. Apart from this she personally helped me many times especially during the initial days of my Ph.D.. I must say, without her help it was actually difficult for me to finish my work in time.

I would like to acknowledge my TIFR friend, Krishnendu Kundu for his personal help and for motivating me to do some paper pen work in theory. I specially thank to UGC for providing me the fellowship as JRF and SRF, which helped me to carry out the research work.

I would like to give my special vote of thanks to three of my labmates: Debarati Bhattacharya, Achintya Dutta and Aryya Ghosh for playing some special role in my Ph.D.. I am highly obliged to Aryya for checking and debugging my intermediate Hamiltonian code with extreme dedication and patience despite his entire busy schedule. This was probably a rate-determining step for my thesis, as that code became a biggest mystery of my Ph.D. life at
that time. Achintya and Debarati were the person whom I used to discuss some idea related to my work, very frequently. In this way, I learned lots of thing from them. The ideas given by Achintya were extremely innovative and helped me to debug my several codes. Achintya had extreme patience to convert any random idea into a productive output in terms of publication, which benefited me also. I think, I should not forget to mention here that the idea of chapter 4 (transition moments in intermediate Hamiltonian) of this thesis originated while discussing and working with Debarati. I specially thank her for this.

I spent a very good time with Sarvesh Ji during the initial two years of my Ph.D. Even after leaving NCL, he is in touch with me and still trying his best to help me whenever I require. I don’t know, what words should I choose to say him “Thank You”.

It is essential to acknowledge two of my special friends Prabhakar Lal Srivastava and Abhishek Mishra for their unconditional help, moral support and critical appreciations at every moment of my Ph.D. life. Prabhakar and Mishra were not only my friends but also much more than that. There are lots of wonderful memories of late night parties also with them. It is difficult for me to express my feelings towards them in few lines, as description about those wonderful moments may transform to several interesting and eventful stories. Let it be for some other pages on some another day.

I am highly thankful to my special friends Atul, Kapil, Prabhakar, Mishra, Pankaj, Prashant, Shameem, Yashwant Sir, Devdutta, Abhijeet Purde and Manish junior and Arvind for making my days eventful in NCL. I am extremely happy and satisfied with the fact that a connection established with some of them in GJ hostel during the weakest moment of my life, is still surviving and becoming more precious day by day. Apart from giving me a company for tea, Atul helped me in writing my papers, typing my equations and improving my presentation slides on almost every occasion during my Ph.D.. Kapil was the person who never denied or postponed anything I requested him. I would like to thank him for this at this stage.
I thank all of my lab mates, Arijit Da, Rahul da, Sumantro Da, Subrato Da, Himadri Da, Bhakti, Tuhina, Lalitha, Deepti, Sapna, Mudit, Sayali, Debarati, Kamalika, Anagha, Shantanu, Achintya, Aryya, Sushanta, Himadri, Manzoor, Turbushu, Sudip, Vidhika, Shaba, Madhulita, Prathit, Aashis, Amrita, Yuvaraj, Jugal, Nisha, Jaya, Manoj and Tamal for providing me a pleasant working atmosphere in the lab during the entire tenure of my Ph.D.

I also thank Mr. Deepak Jori for helping me every time with the administrative issues. I enjoyed talking and debating with Mrityunjay Tiwari about various aspects of society, literature and politics. I was extremely impressed and inspired by some of his masterpiece poems like “Jungle Raaj”. Special thanks to Manzoor and Mudit for personally helping and especially for motivating and pushing me for writing the first draft of my first paper which eventually helped me to get some confidence to go further and finish rest of my Ph.D. work within time frame. It is important to mention some of my friends in GJ hostel namely Kaushal, Anuj, Ajeet, Umesh, Adish, Negi, Prakash, Ankush, Prithwi, Hemender, Ajay, Aanand who gave me a good company at dinner time and helped me during my stay in GJ hostel whenever required. I would like to thank Abhijeet Kayastha, Rupesh, Chaitanya, Krishanu, Brijesh Sharma, Abhimanyu bhaiya, Anjani Dubey, Chetan Sir and Mr. Mane (electric section) for their special appreciation regarding my poetry recitation abilities.

I would like to express my heartiest wishes for all of my NCL audience attending my poetry recitation program and clapping cheerfully during the Research Scholar Meet (RSM) program since last five years.

I have no words to thank my parents “Siya Ram Gupta” and “Kusum Lata Gupta”, my brothers “Bhupendra Gupta” and “Saurabh Agrahari” and my wife “Uma Gupta” for their love, affection, encouragement and unconditional support at every moment of my life.

At last, I express my gratitude to God almighty for his grace.

Jitendra Gupta