Acknowledgements

I would like to thank all the people who have helped and inspired me during my doctoral study. My deepest gratitude goes to my parents, Padmanab and Madhavi, for their love and support throughout my life; this dissertation would have been impossible without them. I am at loss of words for what my father means to me, it is to him that this thesis is dedicated.

Since I joined Professor Gadre’s group for my doctoral studies, I have worked with great number of people whose contribution in assorted ways to the research and the making of the thesis, deserves special mention. It is a pleasure to convey my gratitude to them all, in my humble acknowledgment.

First and foremost I want to thank my guide, Professor Shridhar R. Gadre for his supervision and advice since day one when I joined the Department of Chemistry, University of Pune. His passion for science and “the book of ideas” which lies in his mind, have inspired me as a student. I also adore his fitness, energy and enthusiasm, which is above all of the younger people in his group including me. He has been a fatherly figure for me, always accessible and willing to help. Above all and the most needed, he provided me unflinching encouragement and support in various ways. I am indebted to him more than he knows.

I also wish to express my warm and sincere thanks to my co-guide, Professor Shridhar P. Gejji. I always enjoyed attending his classes and having long discussions with him over variety of topics. Thanks are also due to Dr. P. K. Chaudhury, PKC, as we used to call him, Dr. A. S. Kumbhar and Dr. Sudhir Kulkarni for their words of encouragement.

I have been very fortunate to be a member of the group, rather the family of TCGians. All of my seniors, Ganesh, Balanarayan, Milind and Anant have
pampered me a lot in my early days in the group. I am thankful to them for introducing me to different concepts in quantum chemistry and computational packages. In particular, I owe special thanks to Ganesh for his friendship and patience of tolerating and answering all my silly questions, doubts in the last 5 years. I also especially want to thank Ganesh for teaching me everything I know about linux and Python! Many thanks are also due to Ritwik, Subodh, Sachin for their help in my research. I would like to extend my gratefulness to Nilesh, Kaustubh and Rahul. Thanks are also due to Nityanand, Anmol, Gurmeet, Abhijit and Jonathan for maintaining cheerful atmosphere in lab. I would also acknowledge Sunil and Rohit for all the help and office assistance. My “cousin-labmates”, Moumita, Sujitha and Saurabh have made my stay in IIT, Kanpur, memorable. My warm regards and thanks are due to my friends Vikrant, Dhurba, Trupta, Aruna, Neeta, Priyanka, Ananya, Jaai, Renu, Snehal, Dipti and Mukta.

It is a pleasure to pay tribute to my collaborators: Dr. V. Subramanian and Elango; Dr. S. Sastry and Subha; Professor Sathyamurthy, Brijesh and Ramanathan. I would also like to express my gratitude towards Professor S. Nagase and Dr. Katouda for useful discussions, valuable comments and suggestions on my work during my stay at Institute for Molecular Sciences (IMS), Okazaki, Japan.

I also extend my acknowledgment to Amruta, for being wonderful sister; my beloved little angels Sampanna, Samidha; Vaibhav and Vrushali, for all those fun moments which I will always cherish and all family members including Khandave, Parandekar, Pingale, Natu and Chandekar for their constant encouragement. I wish to express my gratitude to Vishramkaka for all his kind gestures and being my local guardian in Pune and Dr. Autade for helping me out in my difficult days. I would also like to extend my thankfulness to Meenakaku and Apoorva for making
me feel homely during my stay in Japan and Kanpur. I also enjoyed all the time spent in “Bridge club” and long conversations during my stay at their place.

The generous support from Council of Scientific and Industrial Research (CSIR), New Delhi and Centre for Development of Advance Computing (C-DAC), Pune is gratefully acknowledged. Without their financial support this thesis would not be a reality. I would like to express my gratitude towards JENESYS Program and JSPS for providing an excellent platform for researchers in Asia to collaborate, work together, and exchange their views. I also thank Department of Chemistry, University of Pune and Department of Chemistry, Indian Institute of Technology, Kanpur for allowing me to carry out my research.

Anuja