

Acknowledgements

The decision to do Ph.D. has been a life-altering experience for me, and it would not have been possible without the guidance, support, and love that I have received from many people. I take this opportunity to express my sincere gratitude and admiration to all those who made this possible.

First and foremost, I would like to express my sincere gratitude to my supervisor, **Dr. Manikandan Paranjothy**, who introduced me to theoretical chemistry. As a guide, he has given me freedom to participate in academic as well as non-academic activities and been a great support throughout my research work. He is a wonderful person to interact about any issue. His coolest behavior has changed my perception of the Guru-Shishya relationship. I thank him for all the information and the assistance he has provided me throughout five years.

My special words of thanks should also go to my research committee members' Dr. Samanwita Pal, Dr. Atul Kumar, and Dr. Satyajit Sahu, for many fruitful discussions, their valuable advice, and all help regarding my research. It is my great pleasure to have you all in my Ph.D. evaluation committee. I wish to thank Dr. Ritu Gupta for her guidance and for making me feel so comfortable talking about any issue at any time.

I thank all the faculty members of the Department of Chemistry for their support, and for improving my teaching skills through various experimental and theoretical courses. I am overwhelmed with your support and the excellent environment you have provided in the department. I would also like to thank IIT Jodhpur for providing proper infrastructure and research facilities in the institute.

I gratefully thank Yogesh, for all his technical help to start my Ph.D. journey. Without his guidance learning the computational field would not have been so easy for me.

I really appreciate the few people have met at IIT-J, Anchal Gahlaut, Bhawna Chaubey, and Vivek Raghuvanshi, for helping me to make a better version of myself. I thank Shubham, Aditya, and Arpita Srivastava for helping me whenever I needed you with a helping hand or a word of advice. Talking and hanging with you all were the most fun and relaxing moments for me. The last five years here went by so quickly, having you all around.

I owe my deepest gratitude towards my friend Abhishek for his continuous support, care, and belief in me. I am very much indebted to his support in all technical and non-technical fields during my Ph.D. work.

I would like to thank my lab members Erum Gull Naz, Himani Priya, for maintaining a friendly environment at the workspace.

Finally, I would like to appreciate and acknowledge my family members, parents, sisters, and brothers, especially my uncle Shri Maniram Godara who has seen my desire to study at a very young age and provided me an environment to fulfill my dreams.

Sumitra Godara

