

Acknowledgements

tatraika-stham jagat kṛitsnam pravibhaktam anekadhā
apaśhyad deva-devasya śharīre pāṇḍavas tadā
Shrimad Bhagavad Geeta, 11;13

तत्रैकस्थं जगत्कृत्स्नं प्रविभक्तमनेकधा ।
अपश्यद्देवदेवस्य शरीरे पाण्डवस्तदा ॥१३॥

First and foremost my sincere thanks to the "Mighty God", whose existence can be verified by the shloka in Geeta, 11;13 and the concept of Physics "The universe consists of but two elements-matter and energy", where in former Arjun can see the whole universe in one place, in the body of God of gods, and later confirms "God's" presence everywhere. I would like to give full credit for this work to my Ph.D. supervisor Dr. Alpa Dashora. Being the first Ph.D. student, she has supervised me with utmost care and diligence. She has advised me on several research methodologies, teaching skills, and in my career. Her unidirectional approach has kept me in a straight line that kept the workflow, but she has provided me with the freedom to analyze and explore the field on my own which is worth everything. I will always be grateful for your support in helping me develop as a research scientist. I would like to thank my "Grand guide" Prof. B.L. Ahuja, MLSU, Udaipur, who has been my external departmental research committee member and has advised me and motivated me in his ways. I would extend my gratitude to Prof. Krushna Mavani, IIT-Indore, for her role as an external member, and for providing insights into experimental research from the perspective of a computational physicist. I would like to thank Dr. Som Narayan, and Dr. Trupti Gajaria, for being the senior who would direct me towards the conclusion of the research by helping me understand the ways of research techniques. My special thanks go to Kishan Mali, who has been with me on this journey since the very beginning, he

has helped, supported, and helped me learn earlier as an M.Sc student and then as a research colleague. I am heartily thankful to Rushikesh Pokar who helped me explore the Wein2k software and the world in an alternating way. I extend my gratitude to the newest member of our lab Ms. Nayana, whose curiosity, enthusiasm to learn everything, and naive nature helped me revise the whole study. My thanks go to our collaborators Dr. Nainesh Patel, Dr. Rohan Fernandez (Christ University, Bangalore), and Dr. Suraj Gupta (Institut "Jožef Stefan, Slovenia) for their excellent collaboration in providing an experimental perspective in the discussions related to photo/electro-catalyst. My sincere thanks to their students, Avani Chundari, Omkar Bapat, Aniruddha Bhide, Nirmala Thorat, Silviya Ramesh, Akash Suryavanshi, Rinku Bhabal, and Sister Anitha for introducing me to the field of photocatalyst synthesis, electrochemical impedance spectroscopy, cyclic voltammetry, and their overall help. My gratefulness is extended to the DST-INSPIRE scheme, for my fellowship as project fellow, The Maharaja Sayajirao University of Baroda for a University Research Fellowship, the University Supported Research Project, and the National Supercomputing Mission (NSM) for providing computing resources for 'PARAM Ananta' at IIT Gandhinagar, which is implemented by C-DAC and supported by the Ministry of Electronics and Information Technology (MeitY) and Department of Science and Technology (DST), Government of India. I would like to thank Dr. Antone Kokalj (Institut "Jožef Stefan, Slovenia), for providing insights into the area of Carbon dioxide and Nitrogen reduction reaction through long and fruitful discussions. I thank Dr. Bhalamurugan Sivaraman (Physical Research Laboratory, Ahmedabad) for introducing me to the field of research in astrochemistry, along with Dr. Rahul Kushwah, Surendra Vikram, Jaykrishna Meka, for their inspiration to direct me into the research career. My fellow summer interns, Shivam Mishra, Aakanksha Gautam, Vraj Patel, Monica Kosumbi, Nandita Kumari, Dinesh Radhakrishnan, Swathi, and Samiksha Bajaj are active in research fields across the world.

I am deeply grateful to (late) Prof. Dinesh Varshney, Prof. Ashutosh Mishra, Prof. A. K. Dutta, Prof. S. N. Kane, and Dr. Ramjanay Chaudhary, from the School of Physics, and CSR-DAE for igniting the spark in the field of condensed matter Physics. My humble thanks to my M.Sc colleagues, Diksha, Madhuri Padole, Shivani Chouhan, Shivani Patel, SHivangi Verma, Shivangi Sharma, Sudipta Sen, Shubham Dey, (Late) Vivek Mishra and all my classmates for their wonderful friendship and their unwavering support whenever I required. I'm deeply thankful to Shivangi Mishra, Diane Frondozo, and Meghna Gureja, who have supported me

in being consistent with my hard work and kept me motivated during the initial period of my research work.

I'm obliged to Prof. Surjit Mukherjee, Prof. P. K. Jha, Prof. P.K. Mehta, Dr. D. G. Rathod, Dr. Keyur Vyas, Dr. B. Shah, Dr. K Jotania, Dr. P. H. Soni, Dr. R Chauhan, Dr. K Chaudhary, and Dr. Debjani Bagchi for their constant support in the academic teaching and research guidance. I am thankful to all my DRC members for giving me critical comments useful for my thesis work. I'm deeply grateful to Dr. Nakul Patel, Dr. Jolly Mary Joy, Dr. Mahatta Oza, Dr. Nimesh Patel, Dr. Ashwini Mahadik, Dr. Shilpa Bhavsar, Dr. Chaitanya Limbarker, Dr. Bhaskar Soni, Dr. S. Bhattacharya, Dr. Paresh Prajapati, Dr. Arpit, Dr. Niketa, Dr. S. Mukherjee, Dr. Maitri Shukla, Hemang Tanna, Naresh Degada, and other TAPs for helping me understand the ways of this University and in helping me with my academic duties. I would also like to thank Parekh Bhai, Jigna Ma'am, Ajit Bhai, Rajesh Bhai, Matruja Bhai, Suresh Bhai, Jadhav Bhai, Mukesh Bhai, Kishor Bhai, Samanta Bhai, Natu Bhai, Apeksha Ma'am and other non-teaching staff, who have taught me the various technicalities of handling practical instruments and administrative work. I would like to thank all the research students, administrative staff, and non-teaching staff of the M. S. University of Baroda, Vadodara, for their kind support and help in every possible way during my Ph.D. study. I especially thank Dr. Sharad Babu Pillai, Dr. Raghottam Sattigeri, Shardul Vadalkar, Saurav Jana, Darshil Chodvadiya, and other research scholars from the CCMP lab over the years who considered me their own for my full tenure. I extend my gratitude to research scholars from another department including Dr. Abhishek Kumar, Dr. Akash Padmlal, Chinmay Dongre, Poonam Mangtani, Krishna Bhutiya, Rifat Khira, Pankaj Sharma, Dhaval Bhatt, Shreya Pandya, Vijay Gupta, Sukanta Saha for "Chai pr Charcha" leading to very fruitful discussions. My hearty thanks to Aman Mourya, Karan Joshi, Pratik Lakhani, Vishwa-jeet Chavda, Hardik Parmar, Brijesh Patel, Praveen Patil, Gunjan, Vikas, Vijay Joshi, Parth Soni, Sachin Joshi for being supportive in every aspect of hostel life and beyond. Above all, I will always be appreciative of my parents for being a constant source of positivity and for teaching me the importance of education while ignoring my flaws and errors. My father, Mr. Rajesh Bhagat, has taught me the value of loyalty and being sincere in my profession, and my mother, Mrs. Harshlata Bhagat, has always pushed me to seek knowledge and education. Finally, I wish to thank all whom I could not include here for their loving support and for keeping faith in me in completing this marvelous journey.