Statement of Purpose

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My curiosity towards materials science grew leaps and bounds under the able guidance of my father. From my novice days, I was eager to learn more about his discipline and the nature of his work. His new job at Applied Materials, the world's most extensive semiconductors and silicon chips manufacturer, piqued me. A quick visit to his laboratory followed, where I learned that this company produced virtually every new chip and advanced display in the world. I was eager to understand the applications of Material Science at a grass-roots level in building efficient, affordable, and sustainable technologies. The pinnacle of these inspirations was my joining the Indian Institute of Technology, Madras, for undergraduate study (B.Tech) in Metallurgical and Materials Engineering.

I regard Materials Science as a well-rounded discipline that dabbles between several topics that find a prominent presence in academia and industry alike. I have strived to improve my understanding of the research temperament that I desired to cultivate, by actively taking up projects throughout my undergraduate.

My first undergraduate research experience was under the guidance of Prof. Parasuraman Swaminathan in my sophomore year. Eager to explore electronic materials, I numerically modelled a silver nanowire-based thin-film heater using MATLAB and COMSOL. Implementing the learnings from Transport Phenomena, I was able to make theory meet practice. Despite having no prior coding experience, I was able to produce accurate computational results well correlated with the experimental results. Based on this work, I successfully presented a poster at IEEE-ICEE 2020 conference hosted by IIT Delhi. I also contributed to the journal article, "Silver nanowire composite-based heater for wearable applications."

Keen to strengthen my mathematical rudiments, I began another project under the guidance of Prof. Parasuraman Swaminathan that aims to explain the Drude Model based on 2D & 3D random walk problems using probabilistic techniques and Monte-Carlo simulations. This being my first independent work, I learnt to balance collaborative and individual work while actively and systematically communicating my ideas to my advisor. An elegant combination of the coursework from Physics of Materials and program-based simulations resulted in good results. I am penning a preprint titled "Simulating drift velocity in the Drude model using a biased random-walk" to share the results of this work with the scientific community.

In my junior year, I tailored my courses to include Computational Methods in Materials Engineering and the Computational Materials Engineering lab. To explore new concepts learnt, I undertook a project under Prof. Sreeram Kalpathy. I investigated the stability of a thin self-rewetting film exhibiting the Quadratic Thermocapillarity effect bounded by a solid substrate subjected to uniform heating. I am co-authoring a rapid communication paper based on this work, "Thermocapillary effects in self-rewetting liquid films." Writing the manuscript myself, I learnt to communicate ideas in a structured fashion and developed the critical skill of scientific writing.

When I studied Molecular Data Science and Informatics under Prof. Tarak Patra, I noticed a paucity in my data science knowledge. I completed numerous courses in Machine Learning and Deep Learning to upskill myself. As a course project, I recreated the work of Luis A.Miccio and Gustavo A.Schwartz, 'From chemical structure to quantitative polymer properties prediction through convolutional neural networks.' Using randomization in the same model, I obtained lower relative errors (less than 4%) than the original work (6%) itself. This project exposed me to interdisciplinary research, a domain that I have yearned to explore. I have since been working on building a universal autoencoder using feature engineering techniques to convert SMILES string to a multi-dimensional continuous representation for quantitative structure-property predictions, mainly glass transition temperatures of polymers.

During the summer of 2021, I sought international project experience by working on a short virtual project under Prof. Wenhao Sun, University of Michigan, Ann Arbor. I studied chemical potential diagrams and

phase boundaries of Metal-Oxygen-Nitrogen systems to find the critical oxygen potentials of decomposition to oxynitrides. This project sharpened my abilities to represent data concisely using skilful programming techniques. The exposure to DFT techniques I gained here played a pivotal role in shaping my interests in Computational Chemistry and I am currently doing a course on Atomistic Modelling.

My goal as a researcher is to apply computational results in conjunction with experiments to solve real-world problems. With this goal, I am currently working on defect prediction and control of additive manufacturing of Nickel-based superalloys as a part of my undergraduate thesis. I aim to predict the likelihood of detrimental phase formation during wire arc and laser additive manufacturing of aero engines and blades. This work hopes to immensely contribute to the repair-blade industries.

I firmly believe that imparting knowledge is a salient quality of a researcher. I have tried to practise these through teaching assistantships. I have been a teaching assistant for three courses- Introduction to Scientific Computing, Computational Materials Engineering Lab, and Computational Methods in Materials Engineering. I assisted professors in preparing the assignments, grading them and supplementing students with mock solutions. With my strong programming and debugging skills, I handled weekly lab and doubt clarification sessions to address difficulties faced by students. I also taught Computational Mathematics with Sagemath on Gradskey, an online learning platform. I conceptualized the teaching material and provided regular programming assignments to students. During my graduate studies, I would like to gain more teaching experience by connecting with more diverse mindsets.

Additionally, I have practised socially conscious leadership by managing student volunteers at the National Service Scheme (NSS) that trained financially disadvantaged students towards competitive exams. As a student volunteer myself, I have served at the blue-cross society and blood donation camps. I have also been voluntarily teaching Sanskrit to students for six years at GGSS, a non-profit organization. Through various extracurricular activities, I have developed a unique culture and a passion for social, communal, and collective causes.

Experiences throughout my undergraduate studies have taught me that research requires curiosity and persistence. Through various projects, I have demonstrated my ability to apply theoretical knowledge to solve practical problems. My consistent performance has led to my significant academic achievements, currently holding the second rank among 47 in my class. My enthusiastic desire to explore Computational Materials Science is strongly backed by theoretical knowledge and practical exposure.

During my graduate studies, I want to gain more research experience and specialize in Computational Materials Science. I want to strengthen my competence for a PhD and a career in research by developing skills to perform independent, innovative, and high-quality research. The various projects have fortified my belief that rigorous academic research can result in ideas that are feasible to be implemented on a large scale and a career in academia most suited for me. As a professor, I want to share my knowledge with the younger generations by assisting them alongside meaningful research, thereby giving back the guidance I have received. My long-term goal as a researcher is to bridge the gap between academic and industrial research by spearheading cutting-edge projects with widespread impact. I see good potential in supercomputing and data science and inspired by the Materials Genome Initiative 2021, wish to pursue a research career in Integrated Computational Materials Engineering (ICME) and Materials Informatics.

I am very interested in the materials research conducted by Prof. ABC using DEF, KLM, and NOP, particularly in XYZ projects. The research by Prof. ABC in the intersection of ABC and EFG is intriguing as well. Working with these outstanding research groups will provide me with an invaluable opportunity to achieve my dream of quality research. With my academic abilities, requisite skills, and relevant research experience, I feel confident to succeed in the ABC program. I look forward to joining the vibrant student community at XYZ.