MIT Statement of objectives - Chemistry

Recent breakthroughs in machine learning promise to revolutionise approaches to theoretical chemistry. I am drawn to the opportunity to leverage the scientific creativity and technical execution that making the most of these developments requires. A year ago, while designing a small algorithm that allowed for the automated prediction of molecules from IR data as a personal project, I realised my true passion lay in academic research. Only there will my curiosity be satisfied by engaging in novel and groundbreaking endeavours with tangible contributions to the world. Guided by your ethos of collaboration and interdisciplinary learning, I envision leveraging the intricacies of theoretical chemistry, focusing on molecular dynamics and strongly correlated materials to address global challenges. This extends to not only assessing the environmental impact of various processes in catalysis but also the development of more sustainable energy technologies. In particular, I firmly believe — having been deeply involved in advocacy and political initiatives in the past — that policy and academia must work together to solve the greatest challenges that we have ever faced in recent history. This motivates my goal of pursuing not only a PhD in Chemistry, but one at MIT in particular, where policy and science intertwine.

My 4 year bachelors with integrated masters in chemistry has given me a strong and well-rounded foundation in all facets of the subject. In particular, I honed my technical writing ability through writing reports for immersive wet and computational labs, winning the Shimadzu Prize for Practical Chemistry, a testament to my exceptional performance within my cohort. Unfortunately, my university explicitly forbids research placements during term time, and extended Covid-19 restrictions in Hong Kong, relative to the UK and USA, limited my ability to pursue internships during academic breaks, during which I had to return home.

As soon as I could, I seized the opportunity in the spring of 2023 to undertake an internship with venture capital firm Vela Partners. I independently developed an n-nearest neighbours algorithm that analysed the social-media interactions of venture capital investors to determine the n most similar investors. Although I initially contemplated a career in industry after graduation, I redirected my freshly acquired algorithm-development skills to theoretical chemistry, where they found their true home. Additionally, the valuable written communication skills I gained allowed me to apply for and receive the Walters Kundert Chemistry Secondment Fund, Ian Walker Memorial Fund and the Keble Association Internship grants. With these grants, I financed my two recent summer research internships — opportunities I secured through ambitious and competitive applications.

The first was in the Theory of Condensed matter group of the University of Cambridge's Physics department under Professor Mike Payne. Facing the looming existential problem of climate change, carbon nanomaterials and particularly monolayer configurations of 2D fullerene networks give rise to promising new materials for photocatalysing water-splitting processes, thereby producing hydrogen for energy production. This groundbreaking research aimed to understand which monolayer form is stable under ambient conditions. I leveraged first-principles density functional theory together with many-body perturbation theory calculations on high performance supercomputers and determined the optimal substructure for this purpose.

In collaboration with another intern, I joined the Quantum Algorithm Grand Challenge Hackathon, making us the only undergraduate team to participate. Our focus was developing an algorithm on quantum computing simulator software to identify the ground state energy of a rotated Fermi-Hubbard Model, which describes the properties of strongly correlated

electron systems. The long-term vision is to employ algorithms, not unlike the one I developed during my internship, for unprecedented materials design, when quantum computers with more than 100 qubits become available. I was responsible for the optimisation of ansatz circuit parameters through the intricate implementation of an Adam optimiser. This involved navigating complex architectures, and I gained a deep understanding of nuances when solving this problem. We successfully managed to create an algorithm that solved for a ground state energy when given an unknown rotated hamiltonian.
I am actively delving into the applications for similar gradient descent optimisation techniques within the domain of machine learning, driven by an interest in their versatility.

Inspired by my role in the hackathon, I began to implement similar methods for solving quantum many-body problems in existing quantum computer simulators within Qiskit. In combining this personal project with other commitments I have learned to view research as a marathon rather than a sprint. The strong grasp of first principle calculations I gained from this internship, in combination with different computing architectures, prepares me well for a PhD in computational chemistry.

My second research placement was at a Hong Kong University spinoff company, Hong Kong Quantum AI under the supervision of Professor Guanhua Chen, on machine learning exchange correlation functionals for density functional theory. The team's focus was to employ machine learning approaches to reach chemical accuracy, particularly in the realm of utilising molecular dynamics for exploring potential energy surfaces in catalysis. I independently spearheaded a critical initiative focused on generating highly accurate CCSD (Coupled Cluster Singles and Doubles) data for a diverse range of molecules, allowing for the validation of our machine-learned functionals. This underscored the critical role that

supplying high quality data plays in supporting the scientific community in performing small-scale machine learning.

Despite lacking formal pure mathematical experience with neural networks, I drew inspiration from pioneering work done by others in the field, focusing on convolutional neural networks and other machine learning models. I undertook an independent study to devise a loss function that combined both energy and density losses. I therefore contributed to the evaluation of the robustness of algorithms developed by the group. Approaching this challenge from a chemical rather than a mathematical background proved immensely valuable, as it informed an interdisciplinary approach which proved highly successful. I seek the opportunities that MIT provides for cross-departmental learnings and I am confident that I would be in the ideal position to bridge the gap between theoretical chemistry and advanced computation.

The final year of my degree is fully research-based.Currently, I am conducting groundbreaking research under the supervision of Professor David Manolopoulos. This was motivated by my fascination with the transformative potential of machine learning approaches to quantum chemistry. My focus is on developing a machine learning algorithm that finds a kinetic master equation for a diverse range of systems. By leveraging exclusively the short-time dynamics of populations and their long-term equilibrium, we can achieve unparalleled predictive capability over all times, reducing computational cost tremendously. In the short space of time since I began my research, I have already been successful in proving this approach for simulating population dynamics in the Fenna-Matthews-Olson complex - a complex that is widely recognized as a benchmark problem in multi-state dynamics. This underscores my approach’s wide-reaching applications to other systems and

my commitment to pushing the boundaries of scientific inquiry. I hope to apply my approach to spin dynamics simulations in the near future and find it exhilarating to be the first in the field to produce tangible results!

I was excited to see Professor Heather Kulik's research focus on machine learning and density functional theory. I would be ecstatic to work in her team and believe that we share the ambition of pushing automation to surpass the limitations of traditional approaches. Her interdisciplinary work within machine learning accelerated materials discovery seamlessly aligns with my previous experiences in Hong Kong, where I collaborated with a dynamic team to contribute to this field on a small scale. Also, I am eager to collaborate with Professor Troy Van Voorhis, as his work in method development for extracting long-time dynamics from short-time information in simulations resonates with my current masters project. This presents an exciting opportunity for mutual learning and knowledge exchange, where I can contribute findings from my current ongoing work. Likewise, the work of Professor Masha Elkin in how predictive analytics applies to catalysis greatly inspires me, especially in how it could contribute to a more energy efficient future, creating a synergistic link on my previous interests in novel materials for energy harvesting.

I desire the opportunity to contribute my expertise in a creative and challenging environment where I will have a tangible impact. Given the ever-evolving landscape we live in, I envision my career spanning across academia, industry, and public policy. Pursuing a PhD will allow me to take an interdisciplinary approach to problem solving in my career. In particular, through the course of studying at MIT, I hope to gain experience that will allow me to develop computational systems which offer the scientific community a more profound comprehension of our world.

Note On Extenuating Circumstances affecting my final section II exam grades (2022/23 Academic Year)

7 exams are administered consecutively within a time frame of 9 days in the 3rd year for chemistry students at my university. During the last four days of my exams, I encountered unexpected medical issues. During the last two of my final exams, I had to leave the exam room early. As a result, I submitted relevant medical paperwork to the university, in light of which one examination was discounted (‘No result’ on transcript) and the other will be reassessed at the end of my fourth year project.