Letter of Motivation

Biology, computer and mathematics are captivating my passion since I was an undergraduate student. I learnt fundamental mathematical skills that hold the modelling and simulation of biological systems including algebra, differential and integral calculus, differential equations, foundations of statistics, fitting mathematical models to experimental data and Monte Carlo sampling for Bayesian inference. Ascetically I extended my knowledge on constructing molecular models employing corresponding geometry, structure optimization through a numerical model with relevant parameters and analysis to give consistency of the results.

I can use imperative Java lineaments for devising GUI applets, performing basic stream I/O and computation of simple algorithms. Development of electronic structure theory, optimizing algorithms using general-purpose graphics processing units (GPGPUs), molecular electronics, graphene and nanotubes electronics, Monte Carlo methods, potential surfaces, force fields and molecular dynamics in complex and biological environments is my vital principle. I have fondness of writing quantum mechanical codes for the simulations applicable to nanoelectronics. Likewise, I am familiar to C++, Python (syntax and semantics to improve the conventional analysis functions) and FORTRAN.

Regarding my academic credentials I can confirm that the two years masters program is equivalent to the International (British, European and American) Bachelor Standard. In Pakistan, two years Bachelor of Science (B.Sc.) is comparable to Certificate of higher education (CertHE) consistent with National Recognition Information Center (NARIC) United Kingdom. Similarly a student who has a B.Sc. Passed class can get an entrance to the Masters of Science (M.Sc.) program in any of the University in a particular subject lusting two years. In University of the Punjab Lahore, the assessment is conducted annually and the results are prescribed in the form of divisions.

My MPhil Degree was comprising two years. The first year was containing two taught semesters. In semester-I, I proceeded with Advance Stereochemistry (CHEM-740), Advance NMR Spectroscopy (CHEM-741), Medicinal Chemistry (CHEM-743) and Advance by Name Reactions (745) as mentioned in MPhil Degree transcript along with GPA and credit hours. In semester-II, I adopted Heterocyclic Chemistry (CHEM-745), Organometallic Chemistry (CHEM-753), Mass Spectrometry (CHEM-751) and Advance Organic Synthesis (CHEM-750), and details are also available through MPhil degree transcript. In developing my thesis; "Synthesis and Characterization of Novel Benzylidines" I have learned the techniques relevant to molecular modelling, X-ray crystallographic diffraction methods and synthesized several novel molecules along with the comparative study of their properties. I have enjoyed being part of a research team in this exciting area of synthesis and modelling with 12 publications.

During my time at the Department of Chemistry at University of Sargodha, I, not only conducted a very successful research but also enhanced my organizational skills by maintaining exact laboratory records, strengthened my concentration to detail by auditing laboratory. During my MSc degree research work, I spent time at Pakistan Council for Scientific and Industrial Research (PCSIR) Laboratories Complex in Lahore where I was liable for performing HPLC in addition to other laboratory techniques. I have familiarity to analysis, synthesis methods in addition to characterization and molecular modelling (based on QM, MM hybrid QM/MM and MD computer simulations). I would very much like the opportunity to discuss further my application for this position.

My fundamental understanding in the atomistic world has made me to present significant scientific contributions. I have a sound affection with the phenomenon of protein folding. I am competent in the development of force fields and Monte Carlo algorithms, to solve challenging problems in precise description of protein quaternary structures. In this year I have focused in molecular dynamics (MD) simulations using the classical Newtonian equations and Brenner potential, and particularly in combined quantum mechanics and molecular mechanics (QM/MM) method development to study the protein-protein interactions in cellular environment. I have also a plain knowledge to the treatment of electron correlation based on Kohn-Sham equations and density functional models, configuration interaction models and Møller-Plesset models by making use of Gaussian-type functions. One of my executions is thermodynamic properties and behaviours of confined fluids in slit-like and cylindrical pores related to adsorption and diffusion studies. I am considerate to direct simulation Monte Carlo (DSMC) method to understand micro flow systems of small gas molecules. My collective knowledge from various virtual experiments is well enough to manage categorized simulation-works.

I believe that I have the relevant qualifications, research track record, and skills required for the AtoSIM master program. I would like to express my heartiest concentration in an anticipated European Master in theoretical chemistry and computational modelling position. As a newsworthy graduate with research in Organic synthesis and modelling, I deem I am an energetic entrant. I adore commencing my AtoSIM master program, and am confident that I would be a beneficial addition.

Sincerely,

Shahbaz Ahmad