Anna Paulish

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Dear Admission Committee,

I am writing to express my interest in the EPFL doctoral program in Mathematics (EDMA).

Throughout my studies, I have been constantly interested in exploring the applications of mathematical tools in various fields such as crystallography, neuroscience, biology, and now material science. I would be therefore very interested in continuing my academic journey in an interdisciplinary research direction and doing my Ph.D. in the "Mathematics for Materials modelling" Group at EPFL under the supervision of Prof. Michael Herbst. The EDMA doctoral program will give me the opportunity to pursue a Ph.D. with an extremely interesting research line while providing me with many learning and professional growth opportunities to become a successful computational scientist.

I got my bachelor's degree in mathematics at the Novosibirsk State University, and I am currently a third-year EPFL master's student in Computational Science and Engineering. I have been awarded a "MARVEL Inspire Potentials" fellowship to do my master's thesis about "Prediction of atomic arrangements in amorphous structures using generative models" in the Theory and Simulation of Materials (THEOS) laboratory of Prof. Nicola Marzari under the supervision of Dr. Martin Uhrin. I am highly enjoying the project because of its unique combination of mathematics and computer science with applications in materials design and discovery.

I found my inspiration in the research at the intersection of mathematics with materials science where I can apply the knowledge I gained through my studies to solve real-world problems. To explore the world of materials further, I discussed a potential Ph.D. project with Prof. Michael Herbst, the leader of the "Mathematics for Materials modelling" Group, about studying and developing numerical methods for Density-Functional Theory (DFT) simulations. The goal of the project is to make the connection between the materials simulations and applications using the power of advanced numerical methods. The innovative and interdisciplinary nature of this project aligns perfectly with my academic background and research inspirations. I am enthusiastic about numerical analysis, numerical linear algebra, and quantum physics, areas that I want to explore further.

I believe that my studies, experience and skills are best suited to make the project a success. I graduated in mathematics, which gave me a solid theoretical foundation. I then moved to a more applied Computational Science and Engineering program at EPFL where I improved my computational skills by taking a range of courses in data science and computer science.

During my studies, I already had many opportunities to sharpen my skills not only in the classroom but also with various experiences in research labs and internships.

From the first year of my bachelor's, I started gaining research experience as Professor Sergey Gromilov accepted me for a research assistant position in his Laboratory of Crystal Chemistry at Nikolaev Institute of Inorganic Chemistry (Siberian Branch of Russian Academy of Sciences). There I became acquainted with X-ray diffraction methods of crystal structure analysis and conducted an analysis of data from X-ray fluorescence experiments for localization and characterization of mineral admixtures in impact diamonds. I implemented a program that models the X-ray intensity distribution over a collimated beam and earned practical experience in C++ programming.

I became passionate about the subject and continued the project from a more mathematical perspective as my bachelor's thesis at Sobolev Institute of Mathematics (Siberian Branch of Russian Academy of Sciences) under the supervision of Dr. Andrey Lomov on the implementation of data approximation algorithms by Cauchy curves. This work gave me the opportunity to combine mathematics and crystal structure analysis, together with programming. I developed a program that allows to describe the X-ray

diffraction peak profile more precisely, which is crucial for the characterization of non-perfect crystal structures in promising composite and nanodefected materials.

In the summer of 2020, I did my internship at the Mathematical Center of Akademgorodok (Novosibirsk, Russia) where I developed algorithms for determining the ploidy of wheat spikes only on the basis of its images (the classical approach to solve this problem is based on expensive molecular genetic methods).

During my first semester at EPFL, I worked as a student assistant and did my semester project in the Group of Computational Neuroscience and AI of Prof. Alexander Mathis, developing algorithms for detecting outliers using unsupervised machine learning methods in labeled images of animals.

For the second semester, I did my internship at Johnson Electric where I was part of the Digital Transformation team and developed ML-based methods for manufacturing and industrial applications that improve cycle time of production, support quality-proofing of manufactured end products, and result in significant savings for the company.

By the end of the first year of my master's, I realized that computational neuroscience or data science in manufacturing applications are not the areas of my greatest research interest, and decided to explore computational materials science. In September 2022 I performed a semester project under the supervision of Dr. Martin Uhrin in the THEOS laboratory of Prof. Nicola Marzari, where I was developing a machine learning model that can predict plausible but novel amorphous structures and became passionate about the research at the boundary of mathematics and materials science.

I believe that materials science plays a crucial role in shaping technological advancements and I am very inspired to apply my interdisciplinary research experience and solid background to contribute to bringing computational materials science to the next level using advanced mathematical methods.

Joining the EPFL doctoral program in Mathematics is thus a natural step for me, one I am prepared to take and for which I am ready to work with all my energy and enthusiasm. Thank you in advance for considering my application, and I look forward to your reply.

Yours faithfully,

Anna Paulish