Background
Density-functional theory (DFT) is one of the most widely employed simulation methods to predict the properties of materials from first principles. An important application is the computational discovery of novel materials, where many thousands of systematic simulations may be performed. In this regime the often highly problem-specific numerical parameters of DFT need to be automatically selected. This is a highly challenging task, which often proceeds by trial and error, i.e. multiple runs of the same simulation where parameters are tweaked until the simulation is successful. This implies not only a considerable waste of computational resources, but also substantially limits the overall throughput with which new materials can be found.

Project goals
In this project you will obtain and combine physical and mathematical insights into the numerical methods of DFT in order to develop algorithmic techniques, which robustly adapt to the simulated material on the fly. For this you will apply and extend existing results in numerical analysis to obtain novel preconditioners (building upon previous work) as well as adaptive basis selection techniques. Your developed methods will be implemented into codes such as the density-functional toolkit (DFTK) as well as the SIRIUS electronic structure library, such that they can be directly tested on cutting-edge materials simulations. In your work you will be closely integrated into the materials simulation activities at EPFL, e.g. within the NCCR MARVEL, and collaborate with physicists, mathematicians and computer scientists from EPFL, Switzerland and abroad.

Candidate profile
- You are highly motivated and want to become an independent researcher in a fascinating interdisciplinary field, working towards faster and more reliable methods for discovering the materials of tomorrow.
- You have a strong sense of autonomy and independence, but also enjoy being part of a diverse team.
- You have completed a Master (or 4-year Bachelor) in physics, mathematics or a related subject. Candidates who will complete their degree within the next months are also welcome to apply.
- Your academic record is strong and underpins your potential to become an excellent researcher.
- You have a broad background in quantum physics, numerical mathematics and computer science or are looking forward to the challenge of acquiring a diverse cross-disciplinary skillset. In any case your willingness to look beyond the borders of your discipline will be key in this project.
- You have a strong interest in numerical methods, their implementation and application to physics and materials simulations. Previous experience in one of numerical linear algebra, high-performance computing or computational physics is highly desirable.
- You enjoy programming and implementing algorithms and have solid experience in an HPC programming language such as C++, Fortran or Julia.
- You are fluent in written and oral English.
- Bonus skills for this application are considerable experience in numerical analysis, quantum physics, solid-state physics or Julia programming.
What is offered

The activities of the MatMat group centre revolve around understanding modern materials simulations from a mathematical point of view – and to come up with ways to make such simulations faster, quantify their errors or make them more reliable. You will become part of a young and energetic team, fully integrated with both the mathematics and the materials institutes as well as multiple cross-disciplinary initiatives, such as the NCCR MARVEL. Guided by your research topic you have the opportunity to grow substantially your background and obtain expertise in theory as well as applications. For this you have access to a stimulating community of researchers at EPFL’s main campus beautifully located at the lake Geneva shore. For disseminating your work funds to attend suitable conferences and workshops as well as potential visits to our collaboration partners all over the world are provided.

The current regulations regarding salary and working conditions of PhD students at EPFL can be found on the websites linked on https://matmat.org/jobs.