PhD or Postdoc Position

Development of generative methods for the inverse design of materials and molecules

A position is available in Grenoble, France, to work on the development of generative models for the inverse design of materials and molecules. The position is funded by the Multidisciplinary Institute of Artificial Intelligence (https://miai.univ-grenoble-alpes.fr/) in the group of Dr Martin Uhrin with co-supervision by Prof Noël Jakse. We are happy to accept applications from candidates seeking a PhD (3 years) or a postdoc (24 months).

Project summary: The focus of the project is on the development of cutting edge machine learning methods whose goal is to predict atomic structures starting with a set of desired properties. This will involve combining generative models (stable diffusion, normalising flow etc) with invariant and equivariant representations of atomic structures and density functional theory workflows that can accurately calculate labels such that the algorithms can learn to improve autonomously. Target applications will range from prediction of amorphous (glassy) solids, to metal-organic frameworks with targeted bandgaps, to molecules for use as electrolytes in next-generation batteries.

Candidate profile: The ideal candidate will have a master's in computer science/informatics, applied mathematics or physics with experience of machine learning and an understanding of statistical methods. Strong programming skills (in e.g. Python, C++, Julia, etc) are highly appreciated as the candidate will be expected to contribute to codes developed within the group that will be widely disseminated and used in collaborations with groups at Grenoble, EPFL (Switzerland) and MIT.

Working environment: A vibrant and highly stimulating environment that is deliberately multidisciplinary in nature, with access to collaborations at both the multidisciplinary institute in artificial intelligence MIAI (https://miai.univ-grenoble-alpes.fr/) and with physicist, chemists and materials scientists at the Materials and Processes Science and Engineering laboratory (SIMAP, https://simap.grenoble-inp.fr/) where the candidate will be hosted. The candidate will be supported to become an expert in machine learning methods and proficient in generation of large databases of materials properties, both highly sought after skills for a future career in academia or industry. They will also have access to an international network of collaborators at MIT, Harvard, EPFL and Microsoft and be encouraged to present their work at international venues.

How to apply: Please send your application as soon as possible (detailed CV, motivation letter, and names and contact of at least two references to be joined eventually for recommendation letters) by email to the two supervisors with the subject "MIAI ML application". If you'd like to discuss before sending a formal application feel free to write directly to
Martin Uhrin (martin.uhrin@epfl.ch)
Noel Jakse (noel.jakse@grenoble-inp.fr)