A 1+1 year postdoc position is available in Grenoble (France) to work in the field of machine learning applied to the study of electronic structure properties and gas separation of metal-organic frameworks. The position is funded by the MIAI Grenoble Alpes (https://miai.univ-grenoble-alpes.fr/) and will start before December 2021.

Background:

The implementation of efficient carbon capture has been proposed as a means of enabling the continued use of fossil fuels in the near term, while renewable energy sources gradually replace our existing infrastructure. The goal of this project is to computationally design optimal MOFs for an energy efficient carbon-capture-and-release. Specifically, an efficient carbon capture and release mechanism will be achieved by employing a change in the affinity for the gas (and thus a change in its uptake) upon an electronic transition induced by external stimuli.

Methodology:

A method combining machine learning and electronic structure simulations (DFT and CASPT2) will be developed, tested and employed to improve the description of the electronic properties of these materials. One of the challenges is to develop a robust ML model that can provide highly predictive structure–property relationship using a small training set of high quality electronic structure simulations constructed by active learning methods. The model will be developed on small molecules and then tested and used on databases of existing MOFs to predict the gas adsorption properties. The postdoc will work together with a PhD student and in collaboration between physicists, chemists and mathematicians located in Grenoble.

Candidate profile:
We look for highly motivated candidates with a PhD degree in condensed matter physics or chemistry and prior experience with computer simulations and a strong interest in computer science, machine learning and coding ; or a PhD in machine learning or statistics and a strong interest in physics. The candidate should have some skills in programming languages (Fortran, C/C++, Python) and Linux.

The deadline for sending your application is September the 15th and interviews will be conducted soon after. Please send your application as soon as possible by email to the three supervisors:

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Emilie Devijver (emilie.devijver@univ-grenoble-alpes.fr)

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