IPVF
UMR 9006
Joint Research Unit

18, boulevard Thomas Gobert
91120 Palaiseau - France
Tél. : + 33 (0)1 69 86 58 60

Job offer

MISSION TITLE	
Internship : Machine learning applied to photovoltaic materials discovery	

POSITION DESCRITPTION

Function	Intern	Reference	
Contract type	Internship	**Duration**	6 months or more
Starting date	?	**Education**	Master 1 or master 2
Working Place	Palaiseau, Paris area (remote work possible)	**Salary**	600€/month

IPVF IN BRIEF

Become an actor of the Energy Transition by joining a team driven by innovation and impact to address today's most decisive challenges.

IPVF - Institut Photovoltaïque d'Île-de-France, is a global Research, Innovation and Education center, which mission is to **accelerate energy transition through science & technology**.
Gathering industrial PV leaders (EDF, Total, Air Liquide, Horiba and Riber) and world-renowned academic research teams (CNRS, Ecole Polytechnique), multi-disciplinary and international IPVF teams conduct research for clean energy technologies. Supported by the French State, IPVF is labelled Institute for Energy Transition (ITE).

IPVF at a glance:
- *An ambitious Scientific and Technological Program: from tandem solar cell technologies to economy & market assessment, state-of-the art characterization, photocatalysis and concepts breakthrough.*
- *A state-of-the-art technological platform: more than 100 tools, located in cleanrooms (advanced characterization, materials deposition, prototypes for fabrication, modelling…).*
- *A high-standard Education program (M.S. and PhD students).*

JOB CONTEXT

In recent years, halide perovskites gained an impressive momentum in the field of solar cells, as they demonstrated quickly a capability to compete with the best ultrapure crystalline materials while being polycrystalline and made with simple chemistry near ambient temperature, and therefore with a potential for low cost processes for solar cells.
Further studies demonstrated that perovskites, in particular lead halide perovskites (HaPs), display self-healing properties [1-2], i.e., they can recover their electronic properties when submitted to intense physical perturbations. The reason for this is postulated but still debated. Moreover, they contain lead, which is hindering the development of the technology for environmental and public health concerns.

The internship aims at identifying variables (physical properties) that could help identifying suitable materials for solar cells, possibly endowed with self-healing properties, as well as lead free candidates.
The work will be based on experimental data obtained from the Materials Platform for Data Science (MPDS) database, accessed through an API access in python.

Data are already available and have been preprocessed to be easily treated with any regular machine learning (ML) algorithm.

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From a machine learning perspective, this problem is challenging notably due to the numerous missing values present in the data set (thousands of materials described by dozens of physical properties). Two main approaches exist for handling such a problem:
- (i) imputing the data to apply already existing (so called regular) machine learning algorithms
- (ii) use some specific machine learning algorithms capable of handling directly missing values. These two approaches will be explored during the internship. Besides, the physical understanding of the variables may be also useful to design imputations methods tailored for this problem.

[1] D.R. Ceratti et al., Adv. Mater. 30, 1706273 (2018),
[2] W. Nie et al., Nat. Commun. 7, 11574 (2016).
[3] J. Josse, N. Prost, E. Scornet, G. Varoquaux, On the consistency of supervised learning with missing values (2019)

MAIN MISSIONS

- Test of various ML algorithms and assessment of their performance and adequacy on already curated data from incomplete experimental database
- Identification and test of relevant descriptors
- Extracting a list of prospective compounds with potential in photovoltaic conversion of solar energy

SOUGHT PROFILE

Knowledge	Know-how	Self-management skills
▪ Statistics ▪ Data Processing	▪ Python programming ▪ English B1	▪ Curious and challenge driven ▪ Autonomous

CONTACT

Cover letter and résumé to be sent to: Erwan Scornet erwan.scornet@polytechnique.edu; Py--Renaudie Alexandre (M.) alexandre.py-renaudie@polytechnique.edu; GUILLEMOLES Jean-Francois <Jean-Francois.GUILLEMOLES@cnrs.fr>