Dr. Florent PAWULA

6 lieu-dit Sérigny
37160 Neuilly-le-brignon
+33688916524
florent.pawula@cnrs.fr
31 years old

Postdoctoral Researcher

Education

<u>2015 – 2018:</u> **PhD** in **Physics - Material Science**, CRISMAT laboratory UMR6508, Université de Caen Normandie/Ensicaen/CNRS, FRANCE.

<u>2014 – 2015:</u> **2ⁿᵈ cycle diploma Nanomatériaux & Caractérisation de pointe**, Université de Sherbrooke, Québec, CANADA.

<u>2013 – 2015:</u> **Master Multifunctional Materials & New Technologies for Energy** (head of the class), Université de Tours, FRANCE.

<u>2013 – 2014:</u> **Academic certificate: Entrepreneurship, Innovation & Strategy**, Université de Tours, FRANCE.

<u>2009 – 2013:</u> **Licence Science de la Matière (BSC)**, Université de Tours, FRANCE.

Research Experience

<u>Apr. 2022 – to date (early Oct.):</u> **Postdoctoral researcher (JSPS grant, Japan Society for the Promotion of Science)**, National Institute for Materials Science (**NIMS**) and Laboratory for Innovative Key Materials and Structures (**LINK** – CNRS/Saint-Gobain/NIMS – IRL3629) with Dr. Takao MORI and Dr. Guillaume LAMBARD (NIMS senior researchers), and with Dr. Jean-François HALET and Dr. David BERTHEBAUD (CNRS senior researchers), Tsukuba, JAPAN.

Machine learning prospection of efficient thermoelectric chalcogenides

- Optimization of chemical composition for substituted-GeTe using active learning assisted by machine learning and Bayesian optimization. Random Forest algorithm based on elementary descriptors only has demonstrated relatively good performances in modeling the thermoelectric properties for ternary and quaternary substituted-GeTe and also for Cu_2ZnSnS_4 Kesterite. Prediction for proposed chemical compositions targeting optimized thermoelectric properties.
- Optimization of synthesis and process parameters for pristine GeTe to improve efficiency using active learning assisted by machine learning and Bayesian optimization. Prediction for proposed synthesis and process parameters targeting optimized thermoelectric properties.

<u>Jan. 2019 – Nov. 2021:</u> **Postdoctoral researcher (LabEx grant)**, Laboratoire de Chimie des Polymères Organiques (**LCPO**) with Prof. Guillaume FLEURY and Prof. Georges HADZIIOANNOU, Université de Bordeaux/CNRS/Institut Polytechnique, Bordeaux, FRANCE.

Polymer thin films and hybrid single crystals for thermoelectric application

- Vapor phase or in-situ polymerization of PEDOT:Tos. Thin films of tens to hundred nanometers thickness. Nanopatterning using block-copolymer mask and plasma. Opto-electronic, magnetic and thermoelectric properties.
- Investigation of transport behavior of hybrid halide perovskites for solar cell and thermoelectric applications. Single crystal synthesis by antisolvent vapor-assisted crystallization. Crystallochemistry characterizations by XRD and TEM (collaboration) and thermoelectric transport measurements from 2K to 350K.

<u>Oct. 2015 – Sept. 2018</u>: **PhD** in **Physics - Materials Science (Ministerial grant)**, supervisors Dr. Sylvie HÉBERT and Dr. Antoine MAIGNAN (CNRS researchers), Cristallographie et Science des Matériaux (**CRISMAT**) laboratory, Université de Caen/CNRS/Ensicaen, FRANCE.

Ruthenium oxides peculiarities probed by Seebeck effect

- The aim of my PhD was to investigate the Seebeck coefficient in several ruthenium oxides presenting different electronic and magnetic backgrounds to better understand their coexistence. Different structures have been investigated: rutile, hollandites, R-type ferrites and perovskites. Evidence of high T Seebeck coefficient protected from band structure considerations in ruthenium oxides has been demonstrated. During this work, I have synthesized bulk samples by solid state reaction and single crystals by vapor transport, determined their structure with X-ray diffraction and investigated their physical properties (magnetism and thermoelectric transport) with different techniques (cf. Skills section).

<u>July – Aug. 2016</u>: **Research Intern,** National Institute of Materials Science (**NIMS**) in Dr. Takao MORI's group, Tsukuba, JAPAN.

Thermal properties of dense hollandites and 2D chalcogenide single crystals

<u>May – Aug. 2015</u>: **Research Intern,** Laboratory of Physical Chemistry of Matter (**LPCM**) of Prof. Armand SOLDERA, Université de Sherbrooke, Québec, CANADA.

Molecular dynamic modelization of thermoelectric polymer

<u>Jan. – Feb. 2014</u>: **Research Intern,** laboratory of Materials, Components & Systems for Energy Efficiency (**GREMAN**) with Prof. Jean-Claude SORET, Université de Tours & STMicroelectronics, Tours, FRANCE.

Crystallochemistry analyses of the multiferroic GaFeO₃ doped with Yb, Cr

Publications

- Nanostructured PEDOT:Tos thin film from block-copolymer lithography − <u>F. Pawula*</u>, S. Perrot, G. Hadziioannou and G. Fleury*, (*submitted to* **J. Mater. Chem. C**, Oct. 2022)
- Discovery of a new lead-based hybrid hexagonal perovskite − <u>F. Pawula*</u>, A. Fakih, S. Pechev, R. Daou, D. Mantione, O. Lebedev, A. Maignan, G. Hadziioannou, S. Hébert* and G. Fleury, (*submitted to* **J. Mater. Chem. C**, Oct. 2022)
- Effect of Bi nanoprecipitates on the thermoelectric properties of Bi-Sb-Te/Sb2O3 nanocomposites − A. Pakdel, A. U. Khan, <u>F. Pawula</u>, S. Hébert, T, Mori **Adv. Materials Inter.** 9, 24, 2200785 (2022)
- PEDOT:Tos electronic and thermoelectric properties: lessons from two polymerization processes − S. Perrot, <u>F. Pawula*</u>, S. Pechev, G. Hadziioannou and G. Fleury* **J. Mater. Chem. C**, 9, 7417-7425 (2021)
- Thermopower in the $A_{1-\delta}M_{2+x}Ru_{4-x}O_{11}$ (M = Co, Mn, Fe) magnetic hexagonal ruthenates − <u>F. Pawula</u>, R. Daou, S. Hébert, D. Pelloquin, J. Jurazec and A. Maignan **Phys. Rev. B** 103 235106 (2021)
- A Review on Conductive Polymers and Their Hybrids for Flexible and Wearable Thermoelectric Applications − G. Prunet, <u>F. Pawula</u>, G. Fleury, E. Cloutet, A. J. Robinson, G. Hadziioannou, A. Pakdel **Mater. Today Phys.** 18(11):100402 (2021)
- Thermoelectric properties beyond the standard Boltzmann model in oxides: A focus on the ruthenates − <u>F. Pawula*</u>, R. Daou, S. Hébert, A. Maignan. In book: **Thermoelectric Energy Conversion** (2021)
- Anisotropic thermal transport in magnetic intercalates Fe_xTiS_2− <u>F. Pawula</u>, R. Daou, S. Hébert, D. Pelloquin , A. Maignan, A. Subedi, Y. Kakefuda, N. Kawamoto, T. Baba, T. Mori, **Phys. Rev. B** 99 085422 (2019)
- Two new magnetic hollandites $A_{1.5}Ru_{6.1}Cr_{1.9}O_{16}$ (A = Sr, Ba): magnetoresistance and thermopower − <u>F. Pawula</u>, S. Hébert, D. Pelloquin & A. Maignan **J. Mater. Chem. C** 7, 86 (2019)

Communications

Sept. 2022: **Oral presentation (international)**: European Conference of Thermoelectricty (ECT 2022), Barcelona, SPAIN.
- *Machine learning guided prospection of efficient thermoelectric chalcogenides* – F. Pawula, B. Srinivasan, T. Mori, J-F. Halet, D. Berthebaud & G. Lambard

Jul. 2018: **Oral presentation (international)**: International & European Conference of Thermoelectricty (ICT & ECT 2018), Caen, FRANCE.
- *The Seebeck coefficient in some Ru oxides – The example of hollandites* – F. Pawula, S. Hébert, D. Pelloquin & A. Maignan

Dec. 2017: **Oral presentation (national):** Groupement d'Intérêt Scientifique Thermoélectricité (GIS), Montpellier, FRANCE.
- *The Seebeck Coefficient in Oxoruthenates* – F. Pawula, S. Hébert, D. Pelloquin & A. Maignan

Oct. 2017: **Oral presentation (international)**: Research workshop on Spin, Charge and Energy Currents in Novel Materials, Hvar island, CROATIA.
- *The Seebeck Coefficient in Low Dimensional Ru Oxides* – F. Pawula, S. Hébert, D. Pelloquin & A. Maignan

Skills

Synthesis methods: **Solid state reaction, vapor transport, anti-solvent vapor-assisted crystallization, spark plasma sintering**.

Characterization techniques: **DRX, Rietveld refinement, MPMS (Quantum Design) SQUID** magnetometer**, PPMS (QD)** Physical Properties MS **(resistivity ρ, Hall effect, AC Transport ρ, Thermal Transport Option** (ρ, S, thermal conductivity κ)**, ACMS), ZEM3** (S & ρ high T) and **LFA** (κ).

Computer: **OriginPro, Highscore, FullProf, LaTeX, Anaconda, Jupyter notebook,** Keynote, Omnigraffle, Mathematica.

Languages: **French** (mother tongue), **English** (fluent), **Python** (fluent) & **Wolfram** (notions).

References

NIMS laboratory, Tsukuba, JAPAN
Dr. Guillaume LAMBARD: +81298604848 lambard.guillaume@nims.go.jp

LINK laboratory, Tsukuba, JAPAN
Dr. David BERTHEBAUD, LINK - CNRS/Saint-Gobain/NIMS: +33658002290
david.berthebaud@cnrs.fr

LCPO laboratory, Bordeaux, FRANCE
Prof. Georges HADZIIOANNOU: +33540002746 hadzii@me.com
Prof. Guillaume FLEURY: +33540003085 guillaume.fleury@enscbp.fr

CRISMAT laboratory, Caen, FRANCE:
Dr. Sylvie HÉBERT: +33231452910 sylvie.hebert@ensicaen.fr
Dr. Antoine MAIGNAN: +33231451306, +33231452634 antoine.maignan@ensicaen.fr