

Liste des travaux

I. Publications

- 1) F. Pawula, S. Hébert, D. Pelloquin et A. Maignan, *Two new magnetic hollandites $A_{1.5}Ru_{6.1}Cr_{1.9}O_{16}$ ($A = Sr, Ba$): magnetoresistance and thermopower*, **J. Mater. Chem. C** 7, 86 (2019), doi : 10.1039/C8TC04518F
- 2) F. Pawula, R. Daou, S. Hébert, D. Pelloquin , A. Maignan, A. Subedi, Y. Kakefuda, N. Kawamoto, T. Baba et T. Mori, *Anisotropic thermal transport in magnetic intercalates Fe_xTiS_2* , **Phys. Rev. B** 99 085422 (2019), doi : 10.1103/PhysRevB.99.085422
- 3) G. Prunet, F. Pawula, G. Fleury, E. Cloutet, A. J. Robinson, G. Hadziioannou et A. Pakdel, *A Review on Conductive Polymers and Their Hybrids for Flexible and Wearable Thermoelectric Applications*, **Mater. Today Phys.** 18(11):100402 (2021), doi : 10.1016/j.mtphys.2021.100402
- 4) F. Pawula, R. Daou, S. Hébert, D. Pelloquin, J. Jurazec et A. Maignan, *Thermopower in the $A_{1.5}M_{2+x}Ru_{4-x}O_{11}$ ($M = Co, Mn, Fe$) magnetic hexagonal ruthenates*, **Phys. Rev. B** 103 235106 (2021), doi : 10.1103/PhysRevB.103.235106
- 5) S. Perrot, F. Pawula*, S. Pechev, G. Hadziioannou et G. Fleury*, *PEDOT:Tos electronic and thermoelectric properties: lessons from two polymerization processes*, **J. Mater. Chem. C** 9, 7417-7425 (2021), doi : 10.1039/D1TC00756D
- 6) A. Pakdel, A. U. Khan, F. Pawula, S. Hébert et T. Mori, *Effect of Bi nanoprecipitates on the thermoelectric properties of Bi-Sb-Te/Sb₂O₃ nanocomposites*, **Adv. Materials Inter.** 9, 24, 2200785 (2022), doi : 10.1002/admi.202200785
- 7) F. Pawula*, S. Perrot, G. Hadziioannou et G. Fleury*, *Nanotextured PEDOT:Tos layers from block copolymer lithography*, **Org. Electron.** 118, 106806 (2023), doi : 10.1016/j.orgel.2023.106806
- 8) F. Pawula*, A. Fakih, S. Pechev, R. Daou, D. Manton, O. Lebedev, A. Maignan, G. Hadziioannou, S. Hébert* et G. Fleury, *Structural, optical and electronic properties of single crystals of 4H lead-based hexagonal hybrid perovskite*, **Phys. Rev. Mater.** 8, 025403 (2024), doi : 10.1103/PhysRevMaterials.8.025403

- 9) F. Pawula, A. Fakih, R. Daou, S. Hébert, N. Mordvinova, O. Lebedev, D. Pelloquin, et A. Maignan, *Multiband transport in RuO_2* , **Phys. Rev. B**, (2024), doi : 10.1103/PhysRevB.110.064432
- 10) F. Pawula*, M. Hamitouche, L. Abbassi, A. Bajan, C. Bourgès, T. Mori, J-F. Halet, D. Berthebaud, et G. Lambard, *Enhancing thermoelectric efficiency of $GeTe$ through process improvement assisted by active learning and Bayesian optimization*, **STAM-Methods**, (2025), doi : 10.1080/27660400.2025.2545174.
- 11) Y. Ling, F. Pawula, R. Daou, B. Fauqué, and K. Behnia, *T-square electric and its thermal counterpart in RuO_2* , **Phys. Rev. Mater.**, (2025), doi: 10.1103/1qnp-fmm8
- 12) F. Pawula*, I. Chantrenne, B. Fontaine, F. Grasset, S. Cordier, R. Gautier, G. Lambard, D. Berthebaud, et J-F. Halet, *From DFT Calculations to Predictive Models: Machine Learning for Seebeck Coefficient Prediction in Molybdenum Chalcogenide Cluster Compounds*, (2026, submitted to **Phys. Chem. Chem. Phys.**).
- 13) H. Le Du, L. Zullo, J. Cordiez, R. Salvatore, G. Marini, M. Hervé, D. Pierucci, S. Sasaki, F. Pawula, E. Janod, C. Bigi, M. Zonno, F. Bertran, T. Jaouen, P. Le Fèvre, M. Calandra, L. Cario, T. Cren and M. D'Angelo, *Tuning the Charge Transfer of Transition Metal Dichalcogenides via Misfit Layer Compounds*, (2026, submitted to **Adv. Funct. Mater.**), arXiv:2605.18317.
- 14) D. Parmar, C. Bourgès, F. Pawula, P. Deniard, O. Hernandez, C. Guillot-Deudon, J-C Crivello, T. Mori, L. Cario, S. Jobic and D. Berthebaud *Optimization of thermoelectric properties of incommensurately modulated layered composite structure $(La_{0.94}S)_{1.14}NbS_2$: The role of Cationic deficiency and Ce substitution in $La_{0.94}S$ layer*, (2026, to be submitted)

• Chapitre de livre

- 1) F. Pawula*, R. Daou, S. Hébert, et A. Maignan, *Thermoelectric properties beyond the standard Boltzmann model in oxides: A focus on the ruthenates*, dans **Thermoelectric Energy Conversion: Theories and mechanisms, materials, devices, and applications** (2021) ELSEVIER-WP, éd. Ryoji FUNAHASHI, ISBN : 978-0-12-818535-3

II. Conférences et séminaires

• Séminaire invité

- 1) F. Pawula, R. Daou, S. Hébert, D. Pelloquin, A. Maignan, G. Fleury et G. Hadziioannou, *L'effet Seebeck d'oxydes de ruthenium et de polymères semi-métalliques*, Université de Tours (avril 2019).

- 2) F. Pawula, *Novel thermoelectric materials assisted by machine learning*, Laboratoire GREMAN (Tours) puis Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC - Paris), (janvier 2023).
- 3) F. Pawula, *Ruthenium oxide peculiarities probed by the Seebeck effect*, Kyoto University (juin 2025).

• **Présentations orales**

- 1) F. Pawula, S. Hébert, D. Pelloquin et A. Maignan, *The Seebeck coefficient in low dimensional Ru oxides*, **Research workshop on Spin, Charge, and Energy Currents in Novel Materials**, Île de Hvar, Croatie (octobre 2017).
- 2) F. Pawula, S. Hébert, D. Pelloquin et A. Maignan, *The Seebeck coefficient in oxoruthenates*, **Journées Nationales de la Thermoélectricité**, Université de Montpellier (décembre 2017).
- 3) F. Pawula, S. Hébert, D. Pelloquin et A. Maignan, *The Seebeck coefficient in some Ru oxides – The example of hollandites*, **International and European Conference of Thermoelectricity**, Centre des congrès de Caen (juillet 2018).
- 4) F. Pawula, B. Srinivasan, T. Mori, J-F. Halet, D. Berthebaud et G. Lambard, *Machine learning guided prospection of efficient thermoelectric chalcogenides*, **European Conference of Thermoelectricity**, Barcelone, Espagne (septembre 2022).
- 5) F. Pawula, L. Abbassi, T. Mori, J-F. Halet, D. Berthebaud et G. Lambard, *Optimizing the process of chalcogenides to enhance zT using active learning and Bayesian optimisation*, **Internationale Conference of Thermoelectricity**, Seattle, États-Uni (juin 2023).
- 6) F. Pawula, T. Mori, J-F. Halet, D. Berthebaud et G. Lambard, *Advancing Chalcogenide Materials Efficiency Through AI-Driven Studies*, **Workshop GDR Chalco**, Rennes, France (mai 2024).
- 8) F. Pawula, A. Fakih, S. Pechev, R. Daou, D. Mantione, O. Lebedev, A. Maignan, G. Hadziioannou, S. Hébert et G. Fleury, *Hybrid Lead Halide Perovskite Single Crystal: Structural, Optical, and Thermal Properties*, **9th Workshop NIMS - UR – CNRS - Saint-Gobain**, Rennes, France (juin 2024).
- 9) J. Cordiez, H. Ledu, F. Pawula, S. Sasaki, N. Gautier, E. Gautron, C. Ragon, O. Hernandez, B. Corraze, E. Janod, T. Cren et L. Cario, *Crystallochemistry and ultrafast dynamics of misfit chalcogenides*, **2nd International Workshop on Ultrafast Spectroscopy and 2D Materials**, Paris, France (janvier 2025).

- 10) F. Pawula, L. Abbassi, T. Mori, J-F. Halet, D. Berthebaud et G. Lambard, *Enhancing efficiency of chalcogenides through process improvement assisted by active learning and Bayesian optimization*, **International Conference on Thermoelectricity**, Sendai, Japon (juin 2025).
- 11) Crystallochemistry and nanoscale defect of substituted misfit chalcogenide, **9th International symposium on structure property relationship in solid state materials** (SPSSM), Nantes, France (juillet 2025).

- **Affiches**

- 1) F. Pawula, S. Hébert, D. Pelloquin et A. Maignan, *The Seebeck coefficient in Ru-ferrite oxides*, **Journée Scientifique de l'Institut de Recherche des Matériaux** (FR3095), Rouen (juin 2017).
- 2) **Y. Kakefuda**, T. Baba, N. Kawamoto, F. Pawula, R. Daou, S. Hebert, A. Maignan, M. Mitome, D. Golberg et T. Mori, *Microscopic thermal conductivity analysis of two-dimensional single crystals*, **International Union of Materials Research Societies – International Conference on Advanced Materials** (IUMRS-ICAM) Kyoto, Japon (août 2017).
- 3) F. Pawula, S. Hébert, D. Pelloquin et A. Maignan, *The Seebeck coefficient in Ru-ferrite oxides*, **NUconvergence 2018: Frontiers in Aerospace Materials**, Northeastern University, Boston, États-Unis (mai 2018).
- 4) F. Pawula, B. Srinivasan, T. Mori, J.-F. Halet, D. Berthebaud et G. Lambard, *Chalcogenide thermoelectric materials prospection assisted by active learning and Bayesian optimization*, **Réunion thématique “De la Matière quantique aux matériaux fonctionnels”** du GDR MEETICC et du GIS THERMO. Collège de France, Paris (janvier 2023).
- 5) C. Bajan, G. Lambard et F. Pawula, *MADGUI: Material Design Graphical User Interface for active learning assisted by Bayesian Optimization applied to materials*, **Réunion thématique : “New challenges in quantum materials: artificial intelligence and ultrafast science”**, Nantes, France (décembre 2023).
- 6) D. Parmar, C. Bourgès, F. Pawula, P. Deniard, O. Hernandez, C. Guillot-Deudon, J-C Crivello, T. Mori, L. Cario, S. Jobic and D. Berthebaud, *Optimization of thermoelectric properties of misfit layered sulfide by compositional tuning*, **International Conference of Thermoelectricity**, Sendai, Japon (juin 2025)