



BAYESIAN OPTIMISATION FOR MATERIALS RESEARCH (the course is taught in English)

OBJECTIVE:

To present the fundamentals and practical application of Bayesian optimisation, particularly for optimising compositions, synthesis parameters, experimental processes or simulation conditions where each new experiment or calculation involves significant cost.

To make combined use of existing data, model predictions and their uncertainties in order to select, in a sequential manner, the most informative experiments or calculations.

By the end of the course, participants should be able to:

- Formulate a materials research problem as a sequential optimisation problem
- Understand the role of the probabilistic model, uncertainty and acquisition functions
- Set up an initial Bayesian optimisation loop based on experimental or numerical data
- Handle composition, process or structural variables, as well as experimental constraints
- Interpret the algorithm's recommendations and assess the progress of the optimisation
- Identify the main limitations and methodological errors, particularly in the presence of limited data, experimental noise or highly correlated variables

PUBLIC:

This course is open to everyone from the public and private sectors:

-  PhD students or postdoctoral researchers
-  Teachers-researcher
-  Researchers / research engineers

PREREQUISITES:

- A personal laptop is essential
- Knowledge of Python is an advantage, but not essential.

PROGRAM:

Monday 23/11 afternoon:

Visit to the GPM: Materials Physics Group

An Introduction to Active Learning and Bayesian Optimisation

- Why use active learning and Bayesian optimisation in materials research
- Formulation of a sequential optimisation problem
- Data, predictive models and uncertainty estimation
- Introduction to probabilistic models and Gaussian processes
- Initial applied examples in materials science

PROGRAM (continued):

Tuesday 24/11 morning: From prediction to experimental decision-making

- The exploration–exploitation trade-off
- Acquisition functions: Expected Improvement, Probability of Improvement, Upper Confidence Bound
- Constructing a complete Bayesian optimisation loop
- Continuous, discrete and categorical variables
- Experimental noise, constraints and impossible experiments
- Exercises and initial practical work

Tuesday 24/11 afternoon: Optimisation of real-world problems in materials science

- Active learning and Bayesian optimisation applied to compositions, processes and experimental parameters
- Constrained optimisation
- Introduction to multi-objective optimisation and Pareto fronts
- Selection of multiple experiments in parallel
- Practical exercises on representative case studies in materials research
- Analysis and interpretation of the recommendations proposed by the algorithms

Thursday 25/11 morning: Full implementation and best practice

- Design of an end-to-end optimisation campaign
- Evolution of the model and its uncertainty over the course of the experimental cycles
- Termination criteria and assessment of progress
- Reproducibility and key methodological errors
- Discussion based on participants' issues
- Summary and outlook

TRAINEUR :



Guillaume LAMBARD :

Senior Researcher at NIMS (Japan),
within the Data-driven Materials Design
Group.

Associate Professor at Kyushu
University. Specialist in artificial
intelligence and machine learning
applied to materials.

SESSION:

GPM : 23-24-November 2026
(Saint Etienne du Rouvray – 76)

DURATION:

2 days (14h)

MODALITY:

Face-to-face

MEALS (payd for):

Ice-breaker dinner on 23/11 (optional)
Lunch on 24 November

Information and registration:

Places are limited (10 max)



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