APPENDIX

2026 Summer internship at the Institut Courtois

Internship 1

Supervisor: Olivier Fontaine, Department of Chemistry
Title: Predicting Surface Properties from Electrochemical Pen Data Using Modeling and Artificial Intelligence

Surface properties (composition, heterogeneity, oxidation state, wettability, electrochemical activity) govern key phenomena in electrochemistry. Our laboratory is developing a new electrochemical pen concept, a device that enables fast, localized electrochemical measurements on surfaces, generating rich experimental maps that are difficult to interpret directly. To fully exploit this data, it is necessary to link electrochemical signatures to the physicochemical properties of the surface.

In this project, the student will build a modeling and machine-learning pipeline to predict surface properties from electrochemical pen signals. The student will be supervised by a postdoctoral researcher at the interface of chemistry, physics, and data science, with a concrete objective: to transform an emerging instrument into a quantitative diagnostic tool for surface characterization.

Internship 2

Supervisor: Alex Hernandez-Garcia, Department of Computer Science and Operations Research
Title: Generative Machine Learning for Materials Discovery

Artificial intelligence and machine learning promise to accelerate the discovery of novel functional materials for sustainability. Recently, an interdisciplinary group at Mila and the Institut Courtois has been developing Crystal-GFN, a generative machine learning model of crystal structures that integrates crystallography and physical insights to guide the creation of candidate crystalline materials with desirable properties and constraints. After promising results on synthetic tasks, the next goal is to extend the model to better address materials discovery challenges, such as electrocatalyst design and the discovery of new solid electrolytes for solid-state batteries. We are seeking students with a background in machine learning and programming to contribute to the development of Crystal-GFN and its applications.

Internship 3

Supervisor: Carlos Silva, Department of Physics
Title: High-Performance Computation of Quantum Dynamics Using Tensor Neural Networks

On timescales of one millionth of one billionth of a second, the behavior of matter is strongly quantum. Our laboratory seeks to understand how macroscopic properties emerge from this behavior using ultrafast light stimuli. To interpret experimental results, we must simulate the quantum dynamics of matter following its interaction with these light flashes. In this project, you will contribute to making these simulations significantly more efficient by using digital tools from artificial intelligence, specifically tensor neural networks. You will be supervised by an experienced research professional and a doctoral researcher, immersed in a dynamic experimental and theoretical research group.

Internship 4

Supervisor: William Witczak-Krempa, Department of Physics
Title: Measurement-Induced Phase Transitions in Quantum Architectures

Phase transitions induced by measurements represent a new class of non-equilibrium transitions in which the nature of quantum measurements plays a crucial role. Spins or qubits are subject to periodic driving, with unitary evolution alternating with measurements. The transition is controlled by varying the fraction of spins being measured. At low measurement rates, evolution induces many interactions, leading to local decoherence (”scrambling”). At very high rates, frequent measurements destroy entanglement. A new state of matter emerges between these extremes. Preliminary studies show that the spatial range of entanglement near the transition far exceeds that in equilibrium. The student will study how entanglement depends on the fraction of measured spins and will use machine learning methods to find measurement patterns that optimize multi-party entanglement. Since these transitions can be realized on current quantum computers, the project may include running quantum circuits on real quantum hardware.

Internship 5

Supervisor: Audrey Laventure, Department of Chemistry
Title: Development of a Data Standardization Methodology for Automated Design of Tandem Photovoltaic Cells

The overall objective of this project is to accelerate the screening of a wide range of process parameters to enable the fabrication of high-performance tandem photovoltaic cells. The project is based on a robotic platform that integrates artificial intelligence tools to implement a closed-loop feedback framework, supported by a dedicated database that links fabrication parameters with the resulting device properties and performance. The goal of this internship is to establish a methodology for standardizing the multimodal data generated, contributing to the development of a robust database.

Internship 6

Supervisor: François Schiettekatte, Department of Physics
Title: AI Model of Multiple Collision and Pile-Up Effects in Rutherford Backscattering Spectrometry

Rutherford Backscattering Spectrometry (RBS) involves bombarding a material with atoms accelerated by millions of volts and measuring the energy of the backscattered atoms to determine the composition of thin films and nanomaterials. While the basic principles are simple and spectra can be simulated in milliseconds, incorporating effects such as multiple collisions and pile-up can increase simulation time to minutes or even hours. This greatly slows the creation of realistic training datasets for neural networks intended to interpret thousands of measurements. The project aims to determine whether an AI model, trained on experimental data and simulations, can reproduce these complex effects and generate realistic simulations in a much shorter time.

Internship 7

Supervisor: Houari Sahraoui, Department of Computer Science and Operations Research
Title: Adaptive Exploration of Plasma Gun Parameters Using GFlowNets

This internship aims to adapt GFlowNets, a reinforcement learning approach, to efficiently explore the parameter space of a plasma gun in order to modify a material’s physicochemical properties toward predefined objectives. The intern will develop a method combining experimental data-driven approaches with theoretical plasma process models. This hybrid approach will accelerate learning, guide exploration toward the most promising parameters, and optimize the process while reducing the number of required experiments.

Internship 8

Supervisor: Mickael Dollé, Department of Chemistry
Title: Automation of a High-Throughput Characterization Technique for High-Throughput Materials Synthesis

High-throughput synthesis of functional materials requires rapid characterization techniques to identify compositions of interest. The goal of this internship is to automate, under Linux, the entire workflow—from data acquisition to computational management on a local server—for a phase-transition analysis technique parallelized using a thermal camera.

Internship 9

Supervisor: Antonella Badia, Department of Chemistry
Title: Development of an AI Co-Scientist to Assist Users During Scanning Probe Microscopy Measurements

This project represents the first component of an AI co-scientist designed to guide users in conducting scanning probe microscopy (SPM) experiments. It focuses on developing a large multimodal language model (MLLM) that encodes domain-specific SPM expertise and interacts naturally with users. The student will assess the ability of different LLMs to integrate textual and visual data from the microscopy environment, including instrumentation manuals, protocols, and log files (text), as well as user-interface screenshots, microscopy images, and spectra (visual). This analysis will identify the most robust architecture for real-time assistance and recommending appropriate measurement conditions.

Internship 10

Supervisor: Pierre-Luc Bacon, Department of Computer Science and Operations Research
Title: Discovery of Low-Climate-Impact Refrigerants Using Language Models and Reinforcement Learning

Refrigerants used in air conditioning and refrigeration often contribute significantly to global warming, creating a need for more sustainable alternatives. This internship builds on Refgen, an existing molecular generation pipeline combining machine learning with physics-based constraints. The goal is to improve the quality of proposed molecules—particularly their stability and synthesizability—while maintaining strong thermodynamic properties. The work includes data preparation and enrichment, adding criteria and predictors (stability, synthetic feasibility), and integrating these into the optimization process. Special emphasis will be placed on evaluation using thermodynamic models (equations of state, thermo-chemical models) and refrigeration cycle simulations.

Internship 11

Supervisor: Delphine Bouilly, Department of Physics
Title: Correlation Analysis in Graphene-Based Nanosensor Assembly

We develop graphene-based nanosensors (GFETs) for detecting biomarkers in personalized medicine. Because these sensors are assembled using complex processes, we seek to understand how a large fabrication parameter space affects performance. In this internship, the student will analyze existing datasets from microscopy, spectroscopy, and electrical measurements to identify correlations between fabrication conditions and performance using data science, image analysis, and machine learning techniques. This internship is intended for students with strong programming skills, an interest in data science, and curiosity for interdisciplinary research problems.

Internship 12

Supervisor: Will Skene, Department of Chemistry
Title: SolarBot: Automating the Future of Clean Energy

Ever wondered how to teach a chip to smell? Join us to build a micron-sized “electronic nose” capable of detecting complex gas mixtures. You will design smart polymer arrays, integrate them into microchips, and read their signals optically—while mastering microfabrication, device engineering, and AI for real-world sensing applications.

Internship 13

Supervisor: Kevin Wilkinson, Department of Chemistry
Title: Machine Learning and Advanced Multivariate Analysis to Identify Manufactured Nanomaterials in the Environment

Our group studies how to detect human-manufactured nanoparticles in the environment to assess environmental risks. This task is challenging because these particles are extremely rare compared with natural particles such as dust or sea salt. We collect massive datasets from air, water, and soil using a specialized instrument that measures the chemical composition of thousands of particles per minute. We use a Python tool called *IsotopeTrack* to analyze these data. This internship aims to improve the software by making it easier to use and better structured, adding advanced statistical analyses and high-quality visualizations, and integrating machine learning to automatically identify manufactured nanoparticles.