Toward Self-Driven Microscopy Exploration for the Characterization of Functional Materials

Claudia M. Bazán [*1 2] **Kirsty Ellis** [*3 2] **Faisal Mohamed** [*3 2] **Ramzi Zidani** [4 2] **Maxime Goulet** [4 2] **Jean-Nicolas Deraspe** [1 2] **Jeanine Looman** [1 2] **Glen Berseth** [3 5 2] **Delphine Bouilly** [6 2 1] **Audrey Laventure** [4 2]

[*]Equal contribution [1]*Institute for research in immunology and cancer (IRIC), Université de Montréal* [2]*Institut Courtois, Université de Montréal* [3]*Mila, Institut québécois d'intelligence artificielle* [4]*Department of Chemistry, Faculty of Arts and Sciences, Université de Montréal* [5]*Department of Computer Science, Faculty of Arts and Sciences, Université de Montréal* [6]*Department of Physics, Faculty of Arts and Sciences, Université de Montréal*. Correspondence to: Claudia M. Bazán claudia.marcela.bazan@umontreal.ca, Glen Berseth glen.berseth@mila.quebec, Delphine Bouilly delphine.bouilly@umontreal.ca, Audrey Laventure audrey.laventure@umontreal.ca.

1. Introduction

Characterization of low-dimensional features in various advanced materials (polymers, semiconductors, nanomaterials, and others) remains a major bottleneck limiting their full exploitation in electronic and optoelectronic devices [1], [2]. Such features of interest (defects, dopants, interfaces, edges) are often sparsely distributed in large and heterogeneous surfaces or volumes, and conventional imaging and spectroscopy techniques are time-consuming and poorly suited for the exploration of such localized features in large spaces of higher dimensionalities.

2. Approach for autonomous exploration

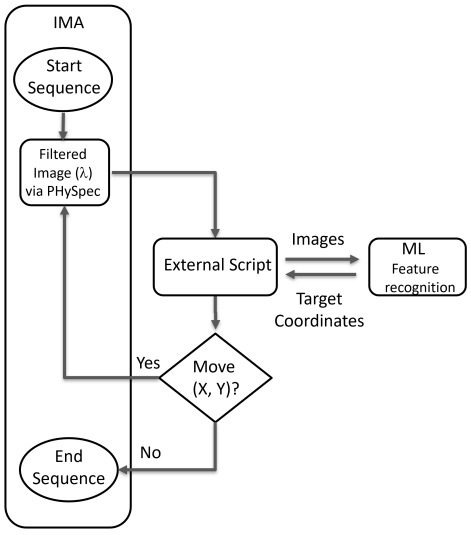

Fig. 1: Workflow for automated exploration: closed-loop for image acquisition and decision-making used to guide subsequent image acquisitions.

We are developing an integrated self-driving laboratory (SDL) approach that combines hyperspectral global imaging systems for Raman (RIMA) and photoluminescence (IMA) with automated workflows to bridge the gap between conventional materials microscopy and intelligent autonomous exploration through closed-loop decision-making. Hyperspectral photoluminescence (PL) mapping using IMA is applied to semiconducting polymer blends and fluorescent dyes, providing spatially resolved insight into their optical and spectral heterogeneity. In a complementary Raman modality, semi-automated filtered RIMA mapping sequences enable large-area imaging of 1D carbon nanotubes (CNTs) dispersed on two-dimensional substrates.

To advance toward autonomy, we report on our recent progress in developing automated navigation and feature-recognition capabilities within the IMA and RIMA platforms (Figure 1). Specifically, we developed a Python-based control framework that interfaces with the IMA system and executes predefined acquisition sequences while autonomously navigating the sample surface. The platform performs randomized stage movements, mimicking human exploratory behaviour, followed by automated image acquisition at target locations. For feature recognition, we implemented an image processing pipeline combining random sampling, image preprocessing, edge detection and filtering to identify CNT features in RIMA images. While this approach demonstrates the feasibility of autonomous navigation and feature-driven exploration, current limitations of the latter include sensitivity to faint edges and noise in edge trajectory prediction.

Ongoing work focuses on improving the robustness of edge detection through deep learning-based approaches and improved initialization strategies. Together, these developments represent a significant step towards transforming PL and Raman spectroscopy into high-throughput, self-driven tools for automated exploration and discovery of complex functional materials.

Acknowledgments

This work was supported by the Institute Courtois through their Exploratory Project grants. The authors thank Professor Richard Martel for access to instrumentation.

References

[1] Delphine Bouilly, Jason Hon, Nathan S. Daly, Scott Trocchia, Sefi Vernick, Jaeeun Yu, Steven Warren, Ying Wu, Ruben L. Gonzalez, Kenneth L. Shepard, and Colin Nuckolls. Single-Molecule Reaction Chemistry in Patterned Nanowells. *Nano Letters*,

16(7):4679–4685, July 2016.

[2] Jiayi Chen, Nahel Blanc, and Audrey Laventure. Towards additive manufacturing of semiconducting polymers: hot-melt extrusion of PCL:P3HT blends. *Materials Advances*, 6(14):4804–4816, July 2025.