AI-Driven Protocol for 2D Materials Growth: Integrating Adaptive Synthesis and Spectral Analysis

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Two-dimensional (2D) materials have emerged as key enablers of next-generation electronic, optoelectronic, and quantum technologies due to their exceptional physical properties [1,2]. However, achieving scalable and reproducible synthesis remains a major challenge. While chemical vapor deposition (CVD) has demonstrated success for certain 2D systems, many materials and heterostructures still lack autonomous, high-throughput fabrication methods that ensure high crystallinity, controlled thickness, and defect minimization at scale. Artificial intelligence (AI) presents a transformative opportunity to optimize these processes [3], not only by accelerating parameter discovery but also by dynamically refining synthesis methodologies through real-time experimental feedback.

We present an AI-driven protocol integrating adaptive Monte Carlo (aMC) optimization with Transformer-based spectral analysis to refine 2D material synthesis. Our autonomous synthesis framework iteratively refines growth conditions, learning time-dependent process parameters without predefined heuristics. The aMC approach generates and executes randomized growth protocols, assessing outcomes via Raman spectroscopy-based feedback. A score function, based on spectral features such as 2D intensity, full-width at half maximum (FWHM) , guides an evolutionary learning process. The system selects, mutates, and refines the best-performing protocols over successive iterations, progressively improving material quality with minimal human intervention [4,5]. A schematic of this workflow is depicted in Figure 1.

Although Raman spectroscopy is a powerful tool for 2D materials [6], conventional peak-fitting techniques struggle with complex heterostructures, where overlapping vibrational modes obscure key features. **To overcome this, we incorporate Transformer-based architectures [7] that use self-attention mechanisms to disentangle spectral components**, extract weak signals, and enhance material evaluation. While our aMC-driven synthesis already functions effectively, integrating AI-enhanced spectral analysis further accelerates optimization, particularly when standard peak-matching fails to provide a clear assessment of material properties.

By combining adaptive synthesis with Transformer-enhanced characterization, we establish a self-refining AI workflow, where synthesis optimization and spectral analysis continuously inform each other. This work demonstrates a clear pathway toward fully autonomous materials laboratories, ensuring scalable, reproducible, and high-quality 2D material production, while accelerating the discovery and application of novel quantum and electronic materials.

References

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Figures

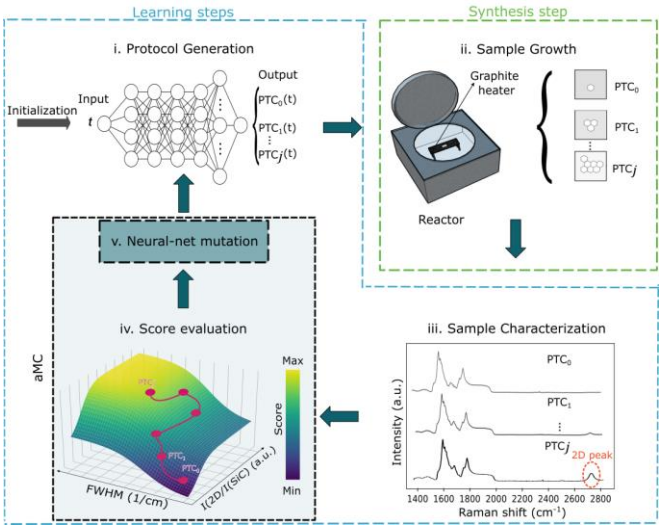

Figure 1. Schematic representation of ANN training used in this work. After initialization with the parameter guess, the protocol generation is conducted (i), followed by sample growth (ii). The sample obtained is then characterized through Raman spectroscopy (iii). The extracted data are used to evaluate the score (iv). Finally, the protocol is updated with the new parameters (v) and a new protocol is generated.

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