Adaptive AI-Driven Material Synthesis: Towards Autonomous 2D Materials Growth

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The advent of artificial intelligence (AI) in materials science heralds a new era of innovative synthesis methodologies. This research explores the frontier of autonomous material synthesis via an artificial neural network (ANN), specifically focusing on the streamlined production of graphene. Our approach is inspired by the work of S. Whitelam and I. Tamblyn who employed evolutionary reinforcement learning for molecular self-assembly[1]. In our work instead we use an adaptive Monte Carlo algorithm for the training of the ANN[2]. This methodology enables the dynamic optimization of the thermal decomposition process of silicon carbide (SiC) into graphene[3], chosen as an ideal testbed due to its simplicity and the limited number of growth parameters (mainly temperature, with pressure held constant).

This study initiates the synthesis process with a random parameter selection within the ANN, which are subsequently refined based on the outcomes of each experimental iteration. At each iteration the ANN proposes a time-dependent temperature protocol (growth recipe). Its performance and adaptability are assessed using Raman spectroscopy, leveraging the graphene Raman fingerprint as a precise metric for evaluating synthesis quality[4]. The scoring system is predicated on the proximity of the Raman signature to that of monolayer graphene, with higher scores awarded to recipes that more closely emulate the ideal monolayer structure. This feedback mechanism is instrumental in the iterative optimization of the ANN's synthesis protocols, progressively enhancing recipe quality. Further validation of the graphene's structural and electronic properties was conducted through supplementary techniques such as atomic force microscopy (AFM), angle-resolved photoemission spectroscopy (ARPES), and X-ray photoelectron spectroscopy (XPS). These analyses provide comprehensive insights into the material quality, affirming the efficacy of the AI-driven synthesis approach.

This research not only demonstrates the viability and advantages of employing AI for material synthesis but also underscores the strategic selection of graphene from SiC as a model system for AI-guided material development. The outcomes highlight the transformative potential of AI in materials science, opening new avenues for discovery and industrial applications. Through the refinement and application of advanced AI methodologies, this work significantly contributes to the progression of materials engineering, promoting a new paradigm of innovation and efficiency in the synthesis process.

References

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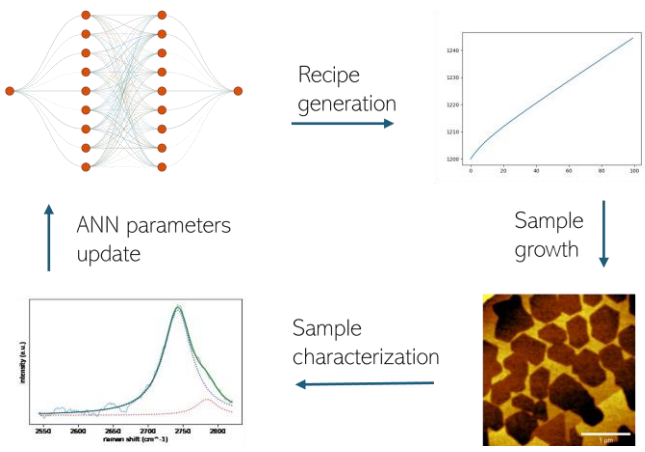

Figure 1. Scheme of the ANN training through score evaluation of the proposed recipes. Once the ANN generates a time-dependent temperature protocol (recipe), the experimental outcome is evaluated via Raman spectroscopy. The distance from the ideal Raman spectrum is translated into a score that serves to update the ANN parameters via an adaptive Montecarlo approach.

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