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Autonomous Matrix Testing and Optimization of 2D Nanocomposites Using Agent-Based Simulation, Computer Vision, and AI

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Abstract

Designing graphene and two-dimensional (2D) nanocomposite matrices typically relies on slow, trial-and-error laboratory testing, manual microscopy inspection, and constant human oversight to tune material parameters. This presentation introduces an autonomous computational framework that combines Agent-Based Simulation and Analysis (ABSA), computer vision, and machine learning to evaluate and optimize 2D material matrices with minimal manual intervention. In this workflow, independent software agents simulate how graphene and 2D fillers disperse and interact within host matrices across varying concentrations, orientations, and environmental conditions. To bridge virtual testing with physical characterization, lightweight computer vision models automatically analyze optical and microscopy imagery to detect filler agglomeration, dispersion uniformity, and structural defects such as wrinkles or voids. Rather than requiring an engineer to manually configure simulations and inspect every sample, the AI-driven ABSA loop continuously integrates visual feedback to generate new test cases, flag performance failures, and converge on optimal matrix configurations. Using benchmark composite and 2D microscopy datasets, this closed-loop approach reduces screening time while uncovering high-performing material combinations that manual workflows often miss. Finally, practical steps for deploying autonomous agent-based and vision-assisted testing pipelines on standard computing hardware are outlined, offering researchers an accessible, hands-off pathway to accelerate 2D nanocomposite development.

Biography

Maalik Khaial is a Nanotechnology Engineering candidate at the University of Waterloo specializing in computational modeling, applied machine learning, and intelligent automation systems. His engineering background spans reactor components and thermal systems modeling at AtkinsRéalis, alongside full-stack software and AI development at Goodself and BirdBrains. His current work focuses on combining autonomous AI agents, simulation workflows, and computer vision to accelerate nanomaterials testing and design.