Opportunities in experimental ai-driven high-throughput materials research

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Resumen:

Artificial intelligence (AI), when paired with laboratory automation, can greatly accelerate materials optimization and scientific discovery. For example, it can be used to efficiently map a phase-diagram with intelligent sampling along phase boundaries, or in 'retrosynthesis' problems where a material with a target structure is desired but a synthetic route is not known. These approaches are especially promising in soft matter and polymer physics, where design parameters (e.g. chemical composition, MW, topology, processing) are vast and where properties and function are intimately tied to molecular design features. However, for AI algorithms to operate efficiently in these spaces, they must also be 'encoded' with relevant domain expertise specific to the problems being tackled. This talk will cover recent advances in hardware and software tools for accelerated materials optimization for polymers and soft matter systems. Finally, it will outline remaining challenges in practical implementations and identify future opportunities for research.