화학과 세미나

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Beyond Self-Driving Labs: Agentic AI and the Future of Autonomous Materials Discovery

Self-driving laboratories (SDL) are rapidly transforming the way scientific research is conducted, enabling accelerated discovery through closed-loop experimentation, data-driven decision-making, and intelligent experimental design. However, many existing autonomous research systems remain limited by synchronous workflows, sparse data, delayed feedback from characterization, and the complexity of real-world experimental processes.

In this talk, I will present our advances toward developing next-generation SDLs powered by Small Science Agentic Models (SSAMs), a modular, domain-specific agentic AI framework designed to integrate scientific reasoning with autonomous experimentation. Rather than relying on general-purpose AI agents, SSAMs employ specialized scientific agents that collaborate to generate hypotheses, design experiments, interpret characterization data, make machine learning-guided decisions, and orchestrate laboratory workflows. By maintaining awareness of the complete experimental trajectory and incorporating physics-informed decision-making under asynchronous conditions, the framework enables more efficient exploration of complex materials design spaces.

I will also discuss our broader vision for autonomous materials discovery, including the integration of domain knowledge, interpretable machine learning, multimodal characterization, and laboratory automation to enable intelligent, adaptive experimentation. Examples from our work on halide perovskites will illustrate how agentic AI can accelerate scientific discovery while providing fundamental insights into structure–property relationships.

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Host : 연세대학교 화학과