[Energy Distinguished Lecture Series]

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High-Throughput Exploration of Chemical Spaces in Halide Perovskites: From Bespoke Synthesis to Designing New Experimental Workflows

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Abstract

Halide perovskites (HPs) offer exceptional compositional and structural diversity that offers a versatile tunability in optoelectronic properties, making them a bespoke materials platform for various optoelectronic applications. Nevertheless, the inherent chemical complexities in the materials result in uncontrolled chemical heterogeneities in the synthesized ensemble system. Specifically, such intricate diversity also creates vast and highly coupled chemical spaces in which phase formation, crystallization, and resulting functionalities are governed by complex interactions among composition, molecular structure, and processing conditions. This not only restricts the full exploitation of their inherited functionalities but also disables the discovery of their genuine synthetic design principle, where challenging these issues requires multidimensional explorations of the synthesis space of the complex materials system. In this talk, I will present our efforts to establish multimodal approaches based on high-throughput automated and autonomous experimentation as a framework pursuing the exploration of these complex synthesis landscapes. Our strategies allow for systematically navigating molecular and compositional spaces, thus enabling us to identify key relationships between molecular structure, formation, and subtle lattice dynamics in inorganic frameworks, and the resulting optoelectronic features and stability. This allows for the discovery of new design principles and processing optimization of perovskites, empowering bespoke customization of their structures, dimensionalities, and functionalities. In addition, I will discuss on how to further understand the chemistry of materials through new, dedicated experimental workflow, which can be automated and autonomously operated to accelerate materials discovery.

Brief Bio



Prof. **Jonghee Yang** is now an Assistant Professor at Yonsei University, South Korea. After receiving Ph.D. degree in Physical Chemistry at Hanyang University, South Korea, in 2020, he worked as a postdoctoral researcher at the University of Tennessee at Knoxville, United States, in Prof. Mahshid Ahmadi's group. His research focuses on the development of high-throughput experimentation to explore chemical and synthesis space of halide perovskites, and experimental-data-driven materials designs with artificial intelligence.

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