Autonomous design of products and processes: Generative Chemical Transformer to reinforcement learning-guided combinatorial chemistry

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Recently, the concept of "autonomous design" has emerged as a way to optimize and design chemical products and processes autonomously. In the field of molecular design, various research achievements have been made from the perspective of inverse design to find molecular structures with desired properties. In this talk, I will introduce the Generative Chemical Transformer (GCT) (*Journal of Chemical Information and Modelling* 61 (12), 5804-5814, Front Cover) that enables high-speed inference while simultaneously matching multiple molecular target properties. At the same time, I mathematically show that extrapolation, a limitation of generative AI, is the same as the problem of predicting extreme properties of molecules. We discuss the methodology and results of reinforcement learning-guided combinatorial chemistry (RL-CC) (*Chemical Science*, 2024, 15, 7908-7925, Front Cover), which was developed to address this problem. Finally, I present the recent applications of RL-CC to (1) non-PFAS surfactant design, (2) amine design for reactive capture of carbon dioxide, and (3) OLED materials. In particular, the section on OLED material design introduces a new evaluation methodology based on bond dissociation energy. Our group utilizes self-supervised learning to efficiently predict the dissociation energy of large molecules at the OLED size level, resulting in improved energy predictions compared to existing methodologies. The combination of RL-CC and representation learning based on pre-trained large chemical models is expected to help solve a variety of problems in autonomous design, such as exploring unknown materials and finding optimal reaction conditions to produce them.