Artificial Intelligence and Robotics for Molecular Materials Discovery

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In this talk, I will overview my group's work on the development of methods for the accelerated discovery of molecular materials such as organic flow batteries and organic light-emitting diodes. The design process shares many features with the design of small molecule pharmaceuticals but also has some key differences. I will overview the status of the field and then discuss our work on generative models for inverse molecular design and also Bayesian methods for robotic control of synthesis and characterization for closed-loop discovery.

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