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"How Can AI Help In Material and Molecule Discovery?"

Abstract: Scientific discovery is one of primary factors underlying advancement of human race. However, traditional discovery process is slow compared to the growing need of new inventions, for example, new antibiotic discovery or design of next-generation energy material. Data-driven approaches such as machine learning and especially deep learning have achieved remarkable performance in many domains including computer vision, speech recognition, audio synthesis, and natural language processing and generation in recent years. Those methods have also infiltrated other fields of science including physics, chemistry, and medicine. Despite these successes and the potential to make huge societal impact, machine learning models are still at infancy in terms of driving and transforming scientific discovery. In this talk, I will talk about a closed-loop paradigm to accelerate scientific discovery, which can seamlessly integrate machine learning, physics-based simulations, and wet lab experiments and enable new hypothesis and/or artefact generation and validation thereof. Development and use of deep generative models and reinforcement learning-based methods for designing novel peptides and materials with desired functionality will be discussed. Finally, I will discuss the importance of adding crucial aspects, e.g. creativity and interpretability, to the machine learning models in order to enable and add value to AI-driven discovery.