Quantum and generative machine learning for molecules and materials

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The discovery of new molecules and materials with desired properties is a practical goal of chemical research. A promising way to significantly accelerate the latter process is to incorporate all available knowledge and data to plan the synthesis of the next materials. In this talk, I will present several directions to use informatics and machine learning to efficiently explore chemical space. I will first describe methods of machine learning for fast and reliable predictions of materials and molecular properties, including quantum mechanical energies and forces. With these tools in place for property evaluation, I will then present a few generative frameworks that we have recently developed to allow the inverse design of molecules and materials with optimal target properties, either in the compositional space or structural space. One general challenge in digital discovery is that many of the molecules and materials that are computationally designed are often discarded in the laboratories since they are not synthesizable. I will thus lastly spend some time to talk about the synthesizability of molecules and materials, either by predicting the synthesis pathways (retrosynthesis) or chemical reactivity. Several challenges and opportunities that lie ahead for further developments of accelerated chemical platform will be discussed.