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Towards inverse design in chemistry: from prediction to deep generative models

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Many of the challenges of the 21st century, from personalized healthcare to energy production and storage, share a common theme: materials are part of the solution. Groundbreaking advances are likely to come from unexplored regions of chemical space. A central challenge is, how do we design molecules and materials according to a desired functionality?
In this talk I showcase how we can apply machine learning to a variety of chemical problems centered around two main themes: 1) building data-driven models for prediction and interpretation of molecular properties and 2) generating and optimizing molecules according to properties via deep generative models.

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