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Computational design and optimization of energy materials

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The use of density functional theory (DFT) to understand and improve energy materials for diverse applications – including energy storage, thermal management, catalysis, and photovoltaics – is widespread. The further step of using high throughput DFT calculations to design materials and has led to an acceleration in materials discovery and development. Due to various limitations in DFT, including accuracy and computational cost, however, it is important to leverage effective models and, in some cases, experimental information to aid the design process. In this talk, I will discuss efforts in design and optimization of energy materials using a combination of effective models, DFT, machine learning, and experimental information.