Machine Learning and Raman Spectroscopy for Energy Materials

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Research of recent years found that several types of energy materials exhibit unusual and very interesting structural dynamics at finite temperature. In semiconductors such as halide perovskites and energy storage materials such as solid-state ion conductors, we and others showed that the peculiar motions of the atoms bear great significance for the functional properties of materials. In my presentation, I will discuss that machine learning has become a tool offering unique capabilities to computationally investigate the complex interplay between atomic dynamics and functional properties in energy materials. With a focus on Raman spectroscopy - a non-invasive and fast method available in many laboratories - I will discuss how machine learning accelerates theoretical predictions and boosts synergies between experiment and theory.