# Molecular Excited States Through a Machine Learning Lens

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## ABSTRACT

Theoretical simulations of electronic excitations and associated processes in molecular systems are indispensable for modern fundamental research and technological innovations. Such simulations are, however, notoriously challenging to perform with quantum mechanical (QM) methods. With advances in machine learning (ML), many new avenues opened for assisting molecular excited-state simulations.

In this talk, we track the progress, assess the current state-of-the-art, and highlight the critical issues to solve in the future. We overview a broad scope of ML applications in excited-state research, with a primary focus on molecules. It includes predicting properties directly, improving QM methods for calculating properties, analyzing data, and generating new compounds.

ML allows for faster and accurate calculation of excited-state properties, which can be exploited to simulate spectra and surfaces, perform dynamics, and search for new optoelectronic materials. Data analysis with ML assists in understanding hidden factors influencing photoprocesses, leading to controlling them and establishing new design rules. Automized generation of new compounds with ML further facilitates optoelectronic materials design.