Machine Learning in Predicting Electronic Absorption Properties of Molecules and Materials

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Predicting the excited state properties, such as the HOMO-LUMO or band gaps as well as absorption spectra for materials and molecules using machine learning (ML) models have gained attention from the researchers across the world [1–5]. ML models can help in predicting the local minimum in potential energy landscape, excited properties of materials and molecules in more faster and acccurate way [6,7]. ML applications in this field are broad, with one major branch dedicated to predicting quantum chemistry-level properties from molecular and material structures. A key research direction focuses on the prediction of primary, secondary, and tertiary properties. Primary properties, such as the Hamiltonian and charge density, form the basis for deriving secondary properties, including physical observables like energies, band gaps, and dipole moments. Tertiary properties, particularly in spectroscopy, include computed spectra such as absorption spectra, obtained from transition dipole moments and vertical transition energies.

While numerous studies have investigated ML-based prediction of tertiary properties, a comprehensive assessment of model effectiveness and optimal input representations remains an open challenge. This poster presents a literature overview of existing ML approaches for predicting tertiary properties, exploring different model architectures, feature representations for molecules and materials, and recent advancements in the field. Finally, we highlight current trends, key challenges, and future opportunities in leveraging ML for direct property prediction in computational chemistry.

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