Artificial Spectroscopy

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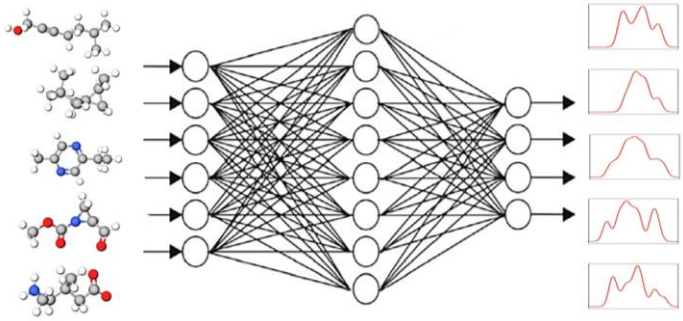
Machine learning (ML) approaches have demonstrated the ability to predict various single-valued properties like melting points, viscosity, corrosion inhibition strength, band gaps, orbital energies, etc. for various types of molecules and materials based on sets of experimental or quantum-computed data. However, continuous data, like spectra (see figure), have not much been in the focus.



Can a machine learn spectroscopy at chemical accuracy?
Is the machine's artificial intelligence able to interpret the spectra?

The first question is clearly answered with yes! We have systematically compared ML models based on different graph neural networks (GNN) in their prediction of excitation spectra from the QM9 data set of organic molecules.[*] Quality measures are the obvious prediction accuracy and runtime measurements, supplemented with a qualitative and quantitative analysis on the impact of different functional.

The second question on the explainability of ML is more difficult to answer. In a current study we analyze the importance of certain atoms – nodes in the GNN – for dominant X-ray transitions of the QM9 molecules and compare it with the participating orbitals obtained from the original quantum-chemistry calculation.

References

[*]K. Singh, J. Münchmeyer, L. Weber, U. Leser, and A. Bande, "Graph Neural Networks for Learning Molecule Excitation Spectra", *J. Chem. Theo. Comput*. DOI: 10.1021/acs.jctc.2c00255 (2022).