Machine Learning Meets Response Properties

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The successes of reduced-scaling coupled-cluster approaches are well known for reaction energies, thermodynamic constants, dipole moments, etc. — properties that depend primarily on the quality of the ground-state wave function. However, much more challenging are higher-order properties such as polarizabilities, hyperpolarizabilities, optical rotations, magnetizabilities, and others that also require accurate representation of the *derivative* of the wave function with respect to external electromagnetic fields. This lecture will provide an overview of our recent efforts to improve the description of such perturbed wave functions, from the development of field-aware densities to streamline local pair-natural orbital methods, to applications of regression techniques to learn the coupled cluster wave function from lower levels of theory, to the use of neural networks for real-time coupled cluster simulations of absorption spectra.