Calculation of Electronic Excited-State Properties via Response Analysis of Perturbed Initial States, and Opportunities for Integration with Artificial Intelligence Research

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Theoretical/computational methods for the computation of (electronic) excited-state dynamics are constantly progressing, largely due to advances in transient spectroscopy and high-performance computing. This talk presents extensions to linear response TDDFT (and wave-function theory in general) to enable calculation of excited-state properties, including absorption spectra of excited states. Our theory is based on the linear-response analysis of perturbed initial states. We discuss applications to organic photovoltaics, and potential integration with artificial intelligence methods to reduce computational costs and to increase exploration of the chemical space.

References: ACS *Energy Lett*. *3*, 155; *J. Am. Chem. Soc*. *139*, 3728.