Combining wave function based Electronic Structure methods and Vibronic Coupling models to simulate electronic spectra.

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In this presentation I will give an overview of theoretical and computational techniques that are being developed in our group (and elsewhere) that aim to simulate electronic spectroscopy for complicated systems like transition metal containing spin systems. The ideal electronic structure method would use localization techniques to enable the study of large systems, combined with explicit r12 techniques to reduce Gaussian basis set requirements. To treat complicated open-shell molecules, e.g. an anti-ferromagnetically coupled bi-metal complex, we use multireference coupled cluster methods. I will speak in particular about our latest development, the MR-EOMCC method, which generalizes single reference equation-of-motion coupled cluster (EOMCC) to the multiconfigurational case. Our eventual aim is to extract vibronic models that describe a limited number of diabatic electronic states, parameterized by a compact set of parameters. In the final step we solve for the (non-adiabatic) nuclear dynamics problem to simulate all features of the spectroscopy. This talk potentially covers a lot of theoretical ground and I will try to convey the essential features.