Valence and Core-Level Excited State Studies of Molecular Complexes and Materials

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In this seminar recent and ongoing developments geared towards studying excited states with linear-response (LR) and real-time (RT) time-dependent density functional theory (TDDFT) will be presented. Over the last decade or so LR-TDDFT has emerged as the method of choice for the calculation of valence excited states of large molecular complexes and materials. However, the method is limited to the linear-response regime. In recent years, RT-TDDFT has begun to emerge as a very promising and computationally efficient approach to model ultrafast electron dynamics and properties that go beyond linear-response perturbations like strong laser pulses. In addition to being able to provide detailed time resolved information, RT-TDDFT can also be used to calculate the optical response of systems with high densities of states like transition metal oxides and large chromophores. I will cover our recent developments in this area and provide an outlook. Finally, recent and ongoing developments and applications in the calculation of pre and near-edge X-ray spectra of molecular complexes and materials will also be presented.