

# Core Excitation Spectra in Attosecond Spectroscopy: A Coupled Cluster Study of FCl

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We have used a variety of methods within the Coupled Cluster family to compute potential energy curves (PEC) of the several core ionized and core excited states of chlorine monofluoride (FCl). The variational collapse of the wavefunction make electronic states involving core holes particularly challenging to describe. Recent extensions in our ground and excited state Coupled Cluster codes have allowed converging such states with ease. In this presentation, we first show the PECs for several core ionized states of FCl, obtained both with a ground state CCSD(T) calculation onto a restricted QRHF reference and with an excited state IP-EOM-CCSD calculation. We compare both approaches and discuss the importance of EOM methods being spin and space eigenfunctions. Secondly, core excited PECs are generated using a projection of EE-EOM-CCSD onto a space of excitations involving at least one core orbitals. These two sets of PEC is finally used to compute the vibronic Hamiltonian and produce photoelectron and core absorption spectra. In our work, we were able to obtain novel PEC for core ionizations and excitations of FCl, which had never been reported before. The ability to obtain potential curves for such elusive states and to generate core absorption spectra opens the door for exciting developments in both theoretical and experimental procedures.