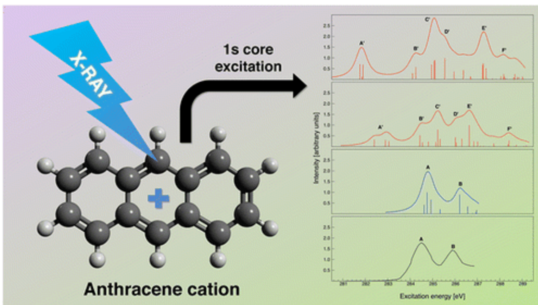
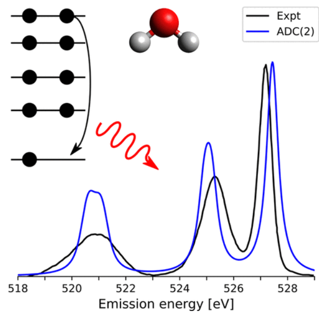
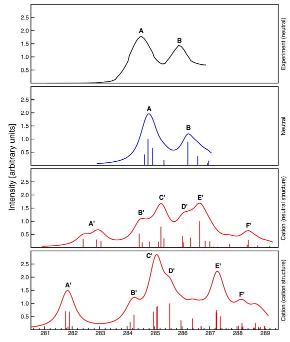
Algebraic Diagrammatic Construction (ADC) Methods for Core-Excited States

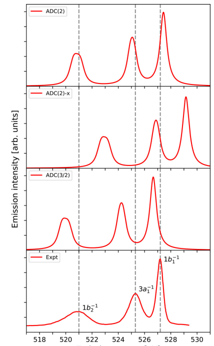




- The algebraic diagrammatic construction (ADC) scheme for polarization propagator is a family of many-body Green's function methods for excited states.
- The ADC expressions can be alternatively derived via the intermediate state representation (ISR). In ISR, the nth order Møller-Plesset (MP) ground state is used as a reference and a correlated excited-state basis set is generated by applying excitation operators to the reference. ADC can be thought of as a MP(n) perturbation theory for excited states.
- The high-lying core-excited states can be accessed by adopting the core-valence separation (CVS) scheme in which the coupling matrix elements between the core and valence orbitals are set to zero.
- ADC provides size-consistent, Hermitian, compact and accurate methods for calculating core-excited states and simulating X-ray spectra.



(a) ADC simulated and experimental carbon-edge XAS of anthracene cation



(b) ADC simulated and experimental oxygene edge XES of water

Request a free trial at www.q-chem.com