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# THE ALGEBRAIC DIAGRAMMATIC CONSTRUCTION FOR THE POLARIZATION PROPAGATOR - A VERSATILE APPROACH TO EXCITED ELECTRONIC STATES, IONIZATION POTENTIALS AND ELECTRON AFFINITIES

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The algebraic diagrammatic construction (ADC) scheme for the polarization propagator provides a series of *ab initio* methods for the calculation of excited states based on perturbation theory. In recent years, the second-order ADC(2) scheme has attracted attention in the computational chemistry community due to its reliable accuracy and reasonable computational effort in the calculation of predominantly singly-excited states. Owing to their size-consistency, ADC methods are suited for the investigation of large molecules. In addition, their Hermitian structure and the availability of the intermediate state representation (ISR) allows for straightforward computation of excited state properties.

In this talk, I will summarize our recent developments in the framework of ADC, which have all been implemented in our *adcman* module as part of the Q-Chem 4.3 program package. These developments comprise ADC(3) for direct computation of excitation energies, ionization potentials and electron affinities of closed and open-shell molecules. The excitation ADC methods have also been adapted to exploit the spin-flip approach to study also ground-state multi-reference molecules, bond-breaking and conical intersections. For the treatment of core-excited states, the core-valence separation (CVS) approximation has also been applied to ADC making efficient CVS-ADC(2) and CVS-ADC(3) programs available. Nuclear excited state gradients are now also available at ADC(2) and ADC(3) level of theory. In addition to the calculation of excited state energies and properties, also an extensive set of density analysis tools are available ranging from standard population analysis tools up to advanced transition density matrix analyses.