Algebraic diagrammatic construction schemes for the calculation of molecular excited, electron-detached and -attached states in complex environments

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Algebraic diagrammatic construction (ADC) schemes received increasing attention during the last two decades, primarily for the investigation of organic photochemistry. In my talk, I will present the intermediate state representation (ISR) formalism to derive ADC calculation schemes for transition energies, state properties and inclusion of external potentials. Recent developments of ADC schemes and the closely related unitary coupled cluster (UCC) methods will be shown and their relation discussed. In particular, the accuracy and usefulness of semi-empirically scaled ADC schemes will be explored. I will also briefly touch upon the potential of ADC methods to compute lifetimes of unbound electronic states and potential energy surfaces for polaritons.