Accurate Green's Functions and Reduced Density Matrices From Algebraic Diagrammatic Construction Theory

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Accurate calculations of reduced quantities such as single-particle Green's functions and density matrices are crucial for computationally efficient and reliable predictions of observables in chemical systems. In this talk, I will present an overview of our group's recent developments in algebraic diagrammatic construction (ADC) theory that enables efficient calculations of Green's functions and reduced density matrices in ground and excited electronic states. This allows to simulate a wide variety of observable properties ranging from excitation energies and spectral functions to electronic density differences and excited-state operator expectation values. I will begin by presenting a brief overview of ADC formalism, highlight the differences between single- and multireference ADC formulations, and demonstrate how these approaches can be used to compute Green's functions and reduced density matrices. My talk will feature applications of ADC to chemical systems with a wide range of electronic correlations.