# Renormalized Propagator Approximations for Calculations on Large Molecules

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Abstract

Efficient, predictive calculations of electron binding energies, double electron binding energies and excitation energies for large molecules are enabled by a new series of approximate electron, two–electron and polarization propagators. Generalizations of second order and renormalized electron propagators that accommodate the fractional occupation numbers of the transition operator method yield excellent results for core as well as valence ionization energies. Improved virtual orbitals that are adapted for specific transitions produce impressive efficiencies in higher–order calculations. New, finite–order methods for the two–electron propagator are capable of aiding assignments of Auger spectra. A combination of finite–order and renormalized self–energies in the polarization propagator yields promising predictions of excitation energies.

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