# Electron Propagator Theory and Correlation–Bound Anions

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## Abstract

Recently developed approximations in *ab initio* electron propagator theory are especially efficient and accurate in calculating electron affinities of molecules and electron detachment energies of anions. This approach involves an energy–dependent, non–local, one–electron operator whose eigenvalues equal electron binding energies that include orbital–relaxation and electron–correlation effects and whose eigenfunctions are Dyson orbitals. Numerical tests of the P3+, NR2 and BDT methods demonstrate their computational and conceptual advantages over other approaches. In addition to providing accurate predictions on various spectral probes of valence–bound anions, these methods also generate precise data on negatively charged species that would not be bound except for strong electron correlation. Examples include newly discovered double–Rydberg anions, diffuse and valence excited states of fullerides and unprecedented kinds of multiply charged species.