

# Correlated Orbital Approximations: Properties of Semiempirical Correlation Potentials

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The objective of this contribution is to introduce the concept of correlated orbital approximations (COAs), which represent a new approach to semiempirical molecular orbital theory (SEMO). In contrast to most semiempirical approaches, COAs are not formally approximations to Hartree-Fock (HF). Instead, semiempirical terms are added to the HF equations in order to include correlation and basis-set effects.

COAs can be understood as an approximation to Bartlett's correlated orbital theory (COT), which introduces correlation in a single particle framework *via* a coupled-cluster self-energy expression. The words theory and approximation are used in this context as in the density functional community: density functional approximations (DFAs) are often designed to fulfill conditions known to be true for exact density functional theory (DFT). Similarly, COAs are designed to fulfill conditions imposed by wavefunction theory. The use of a semiempirical correlation potential (i.e. a self-energy expression) also implies a relationship to electron-propagator/Green's function theory, which will be discussed. However, it should be stressed that COAs are a correlated, MO-like method, not a semiempirical approximation to electron propagator theory (EPT).