Explicitly-correlated calculations of molecular properties and excitation energies

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Explicitly-correlated coupled-cluster CCSD-R12 and CCSD(T)-R12 calculations are computationally demanding and often restricted to relatively small molecules. To be able to apply explicitly-correlated coupled-cluster methods to larger molecules, we have recently started to develop the more economical models MP2-R12, CC2-R12 and CCSD(R12), using auxiliary basis sets (for the resolution-of-the-identity approximation) and Gaussian-damped correlation factors. At the CC2-R12 level, preliminary results for singlet excitation energies will be presented. The analytical calculation of MP2-R12 energy derivatives for the computation of first-order molecular properties will be discussed.