# The State of Computational Quantum Chemistry

Erik Deumens, Quantum Theory Project, University of Florida

An overview is given of the theory and methods that underlie the software used in computational quantum chemistry today. The essence of each method is described and the way the methods are connected is outlined. This we will cover Hartree-Fock, configuration interaction, multi-reference methods, many-body perturbation theory, coupled cluster theory, density functional theory, and R12 methods. Time-dependent methods have grown in importance, first experimentally and then computationally. Examples will be given to illustrate the methods.

The lecture will end by discussing some problems in need of bright minds with a fresh approach to build solutions.