



# QUANTUM MONTE CARLO FOR ATOMS AND MOLECULES

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The class of ab initio techniques known as *Quantum Monte Carlo* (QMC) methods is used in chemistry to elucidate properties of systems governed by the laws of quantum mechanics. One of the most unique aspects of QMC methods is the use of the probabilistic interpretation of the quantum mechanical wavefunction. By not using a purely analytic approximation to the true wavefunction like traditional ab initio approaches, QMC calculations are able to achieve accuracies on par with more expensive methods with less overall computational effort. Because QMC is also a Monte Carlo method, it is possible to estimate a statistical error associated with the calculation; this is unique among commonly practiced ab initio techniques.

This talk will present the background of QMC, including the general motivations and formal development of the method. In addition, examples of the implementation of QMC as a massively parallel method for efficient, accurate calculation of chemical properties related to electronic structure will be presented. This will be done by putting QMC in context with other ab initio techniques and by making comparisons that demonstrate and explain performance differentials in the various methods. A brief discussion of continuing challenges, new directions, and potential applications outside the realm of standard ab initio electronic structure will also be included.