Quantum Monte Carlo for Molecular Systems

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The quantum Monte Carlo method has become recognized for its capability of describing the electronic structure of atomic, molecular and condensed matter systems to high accuracy.[1,2] This talk will briefly outline the method with emphasis on how it contrasts with basis set methods of ab initio quantum chemistry.

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[1]W. A. Lester, Jr. and R. N. Barnett, "Quantum Monte Carlo Methods for Electronic Structure," in "The Encyclopedia of Computational Chemistry," P. v. R. Schleyer; N. L. Allinger, T. Clark; J. Gasteiger; P. A. Kollman; H. F. Schaefer, III; P. R. Schreiner (Eds.); John Wiley & Sons: Chichester, 1998, 3, 1735.

[2]A. Aspuru-Guzik, A. C. Kollias, R. Salomon-Ferrer, and W. A. Lester, Jr. "Quantum Monte Carlo: Theory and Applications to Atomic, Molecular and Nano Systems," in the Handbook of Theoretical and Computational Nanotechnology, eds. M. Rieth and W. Schommers, American Scientific Publishers (2005), p. 643.