

Multi-reference coupled-cluster methods: Three different approaches

Frontiers in Computational and Information Sciences
Seminar Series

Presented by...

Professor Rodney Bartlett

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Abstract Professor Bartlett will discuss the multi-reference problem in coupled-cluster theory, and describe three different approaches for solving the problem. All are compared for cyclobutadiene's auto-isomerization and other multi-reference problems.

Professor Bartlett pioneered the development of coupled-cluster theory in quantum chemistry to offer highly accurate solutions of the Schrödinger equation for molecular structure and spectra. His group is responsible for the widely used ACES program system.

His other research topics include the search for metastable, high-energy density molecules like N₅⁻; non-linear optics; carbon clusters; NMR coupling constants; new correlated quantum chemical methods for polymers and surfaces; *ab initio* density functional theory; and the "transfer Hamiltonian" for large scale quantum mechanical simulations of materials.

More info: <http://www.qtp.ufl.edu/~bartlett/>

Date: February 14

**Location: EMSL
Auditorium**

Time: 1:00 pm