Closed-Shell Coupled Cluster, Excited Electronic States, and Quantum Chemistry Applied to Astrochemistry

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I will discuss some of the research that was done in collaboration with Profs. Gustavo Scuseria and Martin Head-Gordon from 1985 up to the present including some personal anecdotes. The research begins with the first closed-shell singles and doubles coupled-cluster (CCSD) derivation and program, continues through the development of excited electronic state methods and then includes applications of these methods to the spectroscopy of molecules of interest in astrochemistry, with a foray into reaction mechanisms for the formation of prebiotic molecules under various astrophysical conditions. I will use the last few slides to highlight some of the other research that is currently taking place in my group at NASA Ames.