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Under AFOSR support over several years, coupled-cluster (CC) and many-body perturbation theory (MBPT) methods for the accurate inclusion of electron correlation in *ab initio* quantum chemical calculations of molecules have been definitively established as often providing the most accurate results for the electronic structure of molecules and their interactions. Such CC/MBPT methods have been implemented into ACES II, a program system widely used throughout the world for obtaining critical information about molecules and their interactions in the absence of experiment. Our recent reviews ("Coupled Cluster Theory: An Overview of Recent Developments," a Chapter in *Modern Electronic Structure Theory*, ed. D.R. Yarkony, World Scientific Publishing Co, Ltd, Singapore (1995) and "Applications of Post-Hartree-Fock Methods: A Tutorial", in *Reviews in Computational Chemistry*, 5, p. 65, eds. D. Boyd and K. Lipkowitz. VCH Publishers, New York, NY (1994)) can be consulted for a more detailed account of this extensive development. This final report covers the last three years of this work, emphasizing new multi-reference CC approaches plus applications of CC theory to various molecular properties.

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# FINAL REPORT

## Molecular Interactions and Properties with Many-Body Methods

## AFOSR-F49620–93–1–0127

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AFOSR-TR-96-0209

# ABSTRACT

UNIVERSITY OF FLORIDA
F49620-93-1-0127

Molecular Interaction & Properties with Many Body Methods

Under AFOSR support over several years, coupled-cluster (CC) and many-body perturbation theory (MBPT) methods for the accurate inclusion of electron correlation in *ab initio* quantum chemical calculations of molecules have been definitively established as often providing the most accurate results for the electronic structure of molecules and their interactions. Such CC/MBPT methods have been implemented into ACES II, a program system widely used throughout the world for obtaining critical information about molecules and their interactions in the absence of experiment. Our recent reviews ("Coupled Cluster Theory: An Overview of Recent Developments," a Chapter in *Modern Electronic Structure Theory*, ed. D.R. Yarkony, World Scientific Publishing Co. Ltd, Singapore (1995) and "Applications of Post-Hartree-Fock Methods: A Tutorial", in *Reviews in Computational Chemistry*, 5, p. 65, eds. D. Boyd and K. Lipkowitz, VCH Publishers, New York, NY (1994)) can be consulted for a more detailed account of this extensive development. This final report covers the last three years of this work, emphasizing new multi-reference CC approaches plus applications of CC theory to various molecular properties.

**Introduction** A variety of Air Force applications require highly detailed information about atoms, molecules, and their interactions. This information is necessary in problems ranging from chemical laser development, to the detection and identification of rocket plumes, to non-linear optics, electron beam technology, and high density and energy fuels.

The crucial component needed to understand molecular reactions is the potential energy surfaces (PES) that serve to describe the attractions among the atoms and molecules. However, such information is not easy to obtain. In many cases, the most direct approach to obtaining accurate potential surfaces for molecules, and detailed information about their excited states, vibrational spectra, and a wealth of other quantities, is high level *ab initio* solutions of the Schrödinger equation.

However, more so than in most other areas, the ability to provide reliable quantum mechanical results for increasingly large molecules depends critically on improved method development. Whereas supercomputers can enable us to make much larger computations with old methods, the simultaneous development of new methods can increase computational capability by further orders of magnitude. In this regard, many-body perturbation theory (MBPT) methods and their infinite-order coupled-cluster (CC) extensions offer a number of attractive features that the more traditional configuration interaction (CI) approaches lack.

Under AFOSR support, we established these CC/MBPT theories as being among the most accurate available, and developed very efficient and generally applicable computer programs to perform CC/MBPT calculations. Also, we employed these methods for the first time in large-scale *ab initio* calculations of potential energy surfaces. The successes of our original work in this effort have been substantial (see previous AFOSR reports and review articles).

Following a statement of research objectives, we review the recent scientific advances we have made under AFOSR support over the last three years.

**Research Objectives** The overall objectives of this research program for AFOSR included the following:

1. The development of new, more accurate and more efficient *ab initio* quantum mechanical methods based upon coupled-cluster (CC) and many-body perturbation theory (MBPT) for determining molecular properties and potential energy surfaces for molecular interactions.
2. The implementation of these methods into highly efficient, transportable computer programs (ACES II), to enable computations on molecules to be made on an almost routine basis, for a wide variety of different properties.
3. The application of these techniques to a variety of problems that are of interest to AFOSR, and that serve to establish the range of accuracy for CC/MBPT methods.

The underlying goal of our effort is highly accurate first principle quantum mechanical predictions of molecular properties. Such tools are already making possible the determination of dissociation energies, moments, polarizabilities, excitation energies, and vibrational and rotational spectra for molecules to an accuracy that is predictive and comparable to experiment. Furthermore, for transient molecules as occur in rocket plumes, combustion, flame chemistry, and interstellar space that are generally difficult to study experimentally, theoretical calculations provide otherwise inaccessible information. In addition, theoretical work provides the underlying framework to understand innumerable important molecular phenomena and to suggest previously unanticipated solutions to defense related problems. All of the new methods which we developed have been incorporated into our Advanced Concepts in Electronic Structure II (ACES II) program system. The program has been established at Air Force installations for use by other Air Force researchers; at other installations supported by NASA and DOE; and in industry (Ford, Lubrizol, Dupont, etc.).

**Notable Accomplishments (1993–1996)**

Our most recent work on this grant has addressed the theory and application of multi-reference coupled-cluster theory. Items A-C summarize various approaches:

A. Despite the enormous successes of single reference CC approaches, there are still situations where MR-CC methods are recommended. These are usually of two types: bond breaking, particularly for multiple bonds, and complicated open shells such as those for transition metal systems. Previously, all rigorous MR-CC methods required an effective Hamiltonian approach that could suffer from "intruder states" that compromises the convergence of the solution, particularly for global potential energy surfaces. In a recent development, we formulated a very convenient, purely spin adapted MR-CC approach that explicitly resolve this problem for low-spin and complicated open shell situations [26]*[1]. Implementation and application will be made in the future.

B. Another approach to multi-reference problems is offered by our new MR-AQCC (multi-reference, averaged quadratic coupled-cluster) [23, 5]. This approach takes advantage of the simplicity of doing multi-reference configuration interaction (MR-CI) calculations in a configuration basis. No entirely rigorous, linked diagram, many-body approach is possible in a configuration basis, since unlinked diagram cancellation can only be effected at the molecular integral level. However, state specific MR-CI is done routinely. The prime weakness in MR-CI is that it is *not* an extensive, many-body method, which causes rather large errors on the scale of accuracy of concern. In MR-AQCC we introduce a method that (1) uses a configuration basis (2) provides an energy functional so that analytical gradients are readily obtained to search energy surfaces; and (3) approximately introduces unlinked diagram cancellations in an "averaged" way. In comparisons with full CI and other reference results, we demonstrate that MR-AQCC is much more accurate that MR-CI and MR-ACPF (approximate coupled pair functional). It is also much better for small multi-reference spaces than the other two approaches. This makes MR-AQCC the choice for a wide range of highly accurate calculations of potential energy surfaces.

C. Another primary contribution was our introduction of the Generalized Valence Bond Coupled-Cluster (GVB-CC) method [17]. We formulated the problem, implemented it into ACES II, and illustrated it for the prototypical problem of the singlet-triplet splitting in methylene [17]. GVB is the simplest reference function that is qualitatively right for several problems, such as breaking a single band, and other cases when a second double excitation is highly weighted in an electronic state of a molecule. This is the situation with $CH_2$. The ground state has two unpaired electrons, giving a triple-state which is well described by a single determinant reference, while the excited singlet state is more difficult

[1] * References refer to publication list on pages 9, 10.

to describe requiring two determinants. GVB is ideal for the latter case. Since the long controversial energy of the singlet-triplet splitting is quite sensitive to this distinction, our recent development of multi-reference GVB-CC was ideally suited to offering a thorough study. We demonstrate that the best single reference CC methods lead to a difference of about 1 kcal/mol compared to experiment, while GVB-CCSD reduces the error to about 0.2 kcal/mol depending upon the particular GVB orbitals. We also introduce a triples correction GVB-CCSD(T) [17] which further improves agreement.

D. Core-excitation spectra are a fascinating new category of experiment made possible by synchrotron radiation at Brookhaven and the Advanced Light Source at Lawrence Berkeley Laboratory. Unlike conventional electronic spectroscopy, where excitations from about 5–15eV are of interest, core excitations involve energies of several hundred eV. The idea is that an electron in a core atomic orbital of a molecule is excited, but rather than exciting it out of the molecule, which will contribute to its photoelectron spectra; it is trapped into a high lying electronic excited state, which in a simple approximation means it now occupies a previously empty excited orbital. With the emergence of such high resolution experiments, there is a tremendous need for new and better *ab initio* theory to help understand the experimental data.

   We have embarked upon that odyssey, developing "new" electron-attached, coupled-cluster (CC) methods to describe this phenomena [19]. In our method, we first use CC theory to describe the core ionized state, and then use our electron attached variant to *add* an electron back into an excited, empty orbital of the core ion. In this way, we achieve the excitation in two steps, but in a manner where orbital relaxation is fully included via step one.

   We report outstanding results compared to high resolution experiments for $N_2$, $C_2H_4$, $C_2H_2$, CO, and $H_2CO$ [19]. Many important problems can be addressed by these experiments including investigating the breakdown of the Born-Oppenheimer approximation, vibrational structures for highly excited states, and imaging molecules beyond the resolution of the electron microscope. This is a great example of how *new* theory must be developed to describe new experiments.

E. As pointed out by Alan Garscadden, $BCl_3$ has an instrumental role to play in plasma etching of semi-conductors. However, little is known of the molecular physics of $BCl_3$, such as its vibrational and electronic spectra, and that for its decomposition products. Hence, we used the full power of the many CC-based methods we have developed under the support of this grant to answer these questions [27]. This is just a sample of the wealth of predictive information that may be obtained from modern *ab initio* correlated theory

F. A special recent contribution to the field was our formulation and implementation of sixth-order MBPT for electron correlation in molecules [16]. This is the first time such results have been reported. There is a special stability to even-order perturbation approximations, emphasized by the extensive application of fourth order [MBPT(4) or MP(4)] for the last dozen years. Unlike MBPT(3) and MBPT(5), which oscillate widely compared to the exact results, the even orders show good convergence. In fourth order, with a Hartree-Fock reference, single, triple and quadruple excitations are introduced for the first time, in addition to contributions from double excitations. In sixth order, we similarly have the initial contribution of CI–like pentuple and hextuple excitations. Hence, such a method provides insight into the role of higher excitations in the correlation problem that has not been previously available.

Using the structure of CC theory, we readily put the theory and program together in such a way that the whole analysis could be presented in *Chemical Physics Letters* [16]. In comparison with full CI for several small examples, we demonstrate that MBPT(6) correlation energies have an average error of only 1.1 kcal/mol, or comparable to experimental accuracy.

G. Sometime back, Pople and co-workers proposed a simplified form of CC theory they misleadingly termed Quadratic Configuration Interaction (QCI). QCISD is simply an approximation to CCSD, making it a "many-body," extensive, non-variational method like CC, while CI is variational and not size extensive. Hence, the CI designation is totally inappropriate. Despite that, since QCISD agrees with CCSD up to fifth-order terms, for most problems there can be little difference. Since QCISD neglects higher order $T_1$ contributions (in CC theory they occur through $T_1^4$, while in QCISD, only linear terms in $T_1$ are retained); to minimize the error QCISD insists that it use a Hartree-Fock reference, since via Brillouin's theorem, $T_1$ is small and the neglect of higher powers of $T_1$ is more justified. On the other hand, CC theory uses the entire flexibility of the theory, permitting all kinds of non-Hartree-Fock references. For such cases, $T_1^4$, terms are critical to the answers obtained.

   The molecule BeO has the property that even the Hartree-Fock result does not make $T_1$ very small. Consequently, we did a comparative study of QCISD, QCISD(T), CCSD and CCSD(T) [18]. We demonstrated that for IR intensities and polarizabilities that the QCI results are off by orders of magnitude compared to CC results. Further, despite claims to the contrary, there is *no* significant computational advantage to QCI when proper intermediates are defined.

H. It is not well appreciated that standard CC theory offers only one of many potential exponential ansätze for describing the correlation problem. Others include extended (ECC), expectation value (XCC), and unitary (UCC). In this paper [20], we analyze all such methods and by proving a number of theorems, show their interrelationship. We also analyze their comparative computational merits, paying attention to several desiderata. Finally, we introduce a new, strongly connected (SC-XCC) ansatz that serves to offer an excellent compromise for many applications.

I. A principal achievement has been the generalization of the widely used CCSD(T) method to general reference functions [1]. In particular, this advance permits the use of restricted open shell Hartree-Fock (ROHF) references for open-shell systems. The CCSD(T) acronym means that after doing a CCSD, the effect of triple excitations are estimated in a non-iterative, perturbative manner. Previously, all such methods assumed canonical Hartree-Fock orbitals, though this choice is frequently inconvenient. We imposed consistency conditions on this approximation that it have the same orbital invariant properties as CCSD itself; that it be correct through fourth order for any reference; and that it be computationally no worse than an iterative $n^6$ step followed by a single $n^7$ step. This led us to a generalized CCSD(T) that has been shown to be highly accurate [1,7,13].

J. Using our relaxed density formalism, analytical gradients were built upon our generalized CCSD(T), which provides the critically important capability of searching a potential energy surface for equilibrium geometries and transition states [1]. This enables the evaluation of vibrational frequencies and associated IR spectra [13], and other properties. One of importance was hyperfine coupling constants (spin densities) for open shell atoms [8].

K. In our continued generalizations of improved methods for the inclusion of triple and quadruple excitations, we presented the theory and implementation of several new coupled-cluster methods correct through sixth order in the energy [2]. Such methods include the non-iterative methods, CC6SDT[Q] CC6SDT(Q), and the iterative one, CCSDTQ-2. In comparisons with reference full CI results, mean absolute errors were 0.276, 0.303 and 0.151 a.u. respectively. These compare favorably to the full CCSDTQ error of 0.046 a.u., and are substantially improved over fourth-order and various fifth-order corrections.

L. The highly non-linear CC equations have many solutions. Some correspond to excited states while some are purely artifactual. We investigated the nature of such multiple solutions of the CC equations for the prototype $H_4$ system [4]. We found that for excited states, the cluster condition that $T_4 \ll T_2^2/2$ is not necessarily satisfied. Also, the extensivity condition of the ground state CC result may not be shared by the excited state solution, because the underlying perturbation series for the excited states is not necessarily converging [4].

M. Properties other than the energy are conveniently obtained from CC theory via the "Relaxed Density Matrix." This quantity is the non-variational generalization of the usual density matrix associated with CI methods. Using the relaxed density, we studied the effect of relativistic corrections onto the dipole moments of the interhalogen molecules, ClF, BrF, IF, BrCl, ICl and IBr [6]. This required a double perturbation treatment of an electric field (dipole) and the Darwin and mass-velocity terms that introduce relativistic corrections. The relativistic corrections were shown to be essential in obtaining adequate agreement with experiment for the dipole moments [6]. This work is pertinent to the chemical laser based upon the IF molecule.

N. A related study investigated second-order properties, such as those required in the spin-spin coupling constants pertinent to NMR experiments. We evaluated all the terms for the Fermi-contact, spin-dipole, paramagnetic spin orbit and diamagnetic spin orbit parts of the spin-spin coupling constants using the CC method for second-order properties [9]. Whereas for organic molecules the Fermi contact term is dominant, this is not the case for other types of molecules. The average error compared to experiment for several molecules was less than 15% [9].

All of the above are important, timely developments in the field that provide solutions to molecular problems that in many cases, could not be previously addressed.

## Publications Supported by AFOSR-F49620-93-1-0127 (1993-1996)


1. J.D. Watts, J. Gauss and R.J. Bartlett, "Coupled-Cluster Methods with Non-Iterative Triple Excitations for Restricted Open-Shell Hartree-Fock and Other General Single Determinant Reference Functions. Energies and Analytical Gradients," J. Chem. Phys. **98**, 8718 (1993).
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4. L. Meissner, A. Balkova and R.J. Bartlett, "Multiple Solutions of the Single Reference Coupled Cluster Method," Chem. Phys. Lett. **212**, 177 (1993).
5. P.G. Szalay and R.J. Bartlett, "Multi-Reference Averaged Quadratic Coupled-Cluster Method: A Size-Extensive Modification of Multi-Reference CI," Chem. Phys. Lett. **214**, 481 (1993).
6. S.A. Perera and R.J. Bartlett, "Relativistic Effects at the Correlated Level: An Application to Interhalogens," Chem. Phys. Lett., **216**, 606 (1993).
7. J.D. Watts and R.J. Bartlett, "Triple Excitations in Coupled-Cluster Theory: Energies and Analytical Derivatives," Int. J. Quantum Chem. **S27**, 51 (1993).
8. S.A. Perera, J.D. Watts and R.J. Bartlett, "A Theoretical Study of Hyperfine Coupling Constants," J. Chem. Phys. **100**, 1425 (1994).
9. S.A. Perera, H. Sekino and R.J. Bartlett, "Coupled-Cluster Calculations of Indirect Nuclear Coupling Constants: The Importance of Non-Fermi Contact Contributions," J. Chem. Phys. **101**, 2186, (1994).
10. J.D. Watts and R.J. Bartlett, "The Inclusion of Connected Triple Excitations in the Equation-of-Motion Coupled-Cluster Method," J. Chem. Phys., **101**, 3073 (1994).
11. J.D. Watts and R.J. Bartlett, "Accurate Electron Affinities of Small Carbon Clusters," J. Chem. Phys., **101**, 409 (1994).
12. M. Urban, J.D. Watts and R.J. Bartlett, "On the Accuracy of Molecular Properties by Coupled-Cluster Methods for Some Difficult Examples: Oxygen Atom, Iron Atom, and Cyano Radical," Int. J. Quantum Chem. **52**, 211 (1994).
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14. J.D. Watts and R.J. Bartlett, "Coupled-Cluster Singles, Doubles and Triples Calculations with Hartree-Fock and Brueckner Orbital Reference Determinants. A Comparative Study," Int. J. Quantum Chem. **28**, 195 (1994).
15. A. Balkova and R.J. Bartlett, "A Multi-Reference Coupled-Cluster Study of the Ground State and Lowest Excited States of Cyclobutadiene," J. Chem. Phys.,**101**, 8972 (1994)
16. S.A. Kucharski and R.J. Bartlett, "Sixth-Order Many Body Perturbation Theory for Molecular Calculations," Chem. Phys. Lett., **237**, 264 (1995).
17. A. Balkova and R.J. Bartlett, "On the Singlet-Triplet Separation in Methylene. A Critical Comparison of Single versus Two Determinant (Generalized Valence Bond) Coupled Cluster Theory," J. Chem. Phys., **102**, 7116 (1995).

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19. M. Nooijen and R.J. Bartlett, "Description of Core-Excitation Spectra by the Open-Shell Electron-Attachment Equation-of-Motion Coupled Cluster Method," J. Chem. Phys.,**102**, 6735 (1995).
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23. P.G. Szalay and R.J. Bartlett, "Approximately Extensive Modifications of the Multi-Reference Configuration Interaction Method: A Theoretical and Practical Analysis," J. Chem. Phys.,**103**, 3600 (1995).
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25. M. Nooijen, "Many-Body Similarity Transformation Generated by Normal Ordered Exponential Excitation Operators", J. Chem. Phys. **104**, 2638 (1996)
26. M. Nooijen and R.J. Bartlett, "General Spin Adaptation of Open-Shell Coupled Cluster Theory", J. Chem. Phys., **104**, 2652 (1996).
27. K.K. Baeck and R.J. Bartlett, "*Ab Initio* Study for $BCl_3$ Plasma: Structure, Spectra and Decomposition Paths," J. Chem. Phys., to be published.

## Invited Presentations Assisted by AFOSR-F49620–93–1–0127 (1993–1996)

1. December 1993 — "Quantum Chemistry of Relevance for the US Department of Defense," Stockholm, Sweden
2. December 1993 — Symposium on Molecular Interactions, Aarhus University, Aarhus, Denmark
3. November 1993 — Nagoya Symposium on Chemical Reaction Theory, Nagoya University, Nagoya, Japan
4. August 1993 — 206th National Meeting of the American Chemical Society, Chicago, Illinois
5. July 1993 — International Academy of Quantum Molecular Science, Menton, France
6. June 1993 – First Congress of the International Society for Theoretical Chemical Physics, University of Girona, Girona, Spain
7. May 1993 — AFOSR/NE Atomic, Molecular and Plasma Physics Workshop, Dayton, Ohio
8. May 1993 – 11th Robert S. Mulliken Lecturer, University of Georgia

9. May 1994 — "Excited States in Coupled–Cluster Theory: Valence, Rydberg and Core Excitations," 2nd Canadian Computational Chemistry Conference, Kingston, Ontario, Canada
10. June 1994– "Properties in Coupled Cluster Theory," 8th International Congress of Quantum Chemistry Satellite Meeting, Bratislava, Slovakia
11. June 1994 — "Coupled Cluster Theory as a Unified Approach to Molecular Spectra," 8th International Congress of Quantum Chemistry, Prague, Czech Republic
12. October 1994 — "Coupled Cluster Theory as a Unified Approach to Molecular Spectra," Workshop on Non-Perturbative Many Body Methods (From Quantum Field Theory to Chemistry)," Bad Honnef, Germany
13. May 1995 — "Equation of Motion Coupled Cluster Methods with Application to $BCl_3$," Air Force Office of Scientific Research Contractors Meeting, Wright-Patterson AFB, CA
14. May 1995 — "Equation of Motion Coupled Cluster Methods for Excited, Ionized and Electron-Attached States," Pople Symposium, Northwestern University, Evanston, IL

## Students Partially Supported by AFOSR-F49620–93–1–0127

1. Mr. Sullivan Beck
2. Dr. David Bernholdt, Ph.D. 1993
3. Dr.. S. Ajith Perera, Ph.D. 1996
4. Mr. Piotr Rozyczko
5. Ms. Lynn Salemi
6. Mr. Steve Gwaltney

## Postdoctoral Research Associates Partially Supported by AFOSR-F49620–93–1–0127

1. Dr. Anna Balkova
2. Dr. Leszek Meissner
3. Dr. John Watts
4. Prof. Stanislaw Kucharski
5. Prof. Miro Urban
6. Dr. Marcel Nooijen
7. Dr. Peter Szalay

## 6. Professional Honors

Bartlett, Rodney, J, Fellow, International Academy of Quantum Molecular Sciences, Menton, France, 1991

Bartlett, Rodney, J, 18th most cited chemist in the world for the 1984–1990 period, Science Watch Magazine, May, 1992.

Bartlett, Rodney, J, American Physical Society, Fellow, November, 1989

Bartlett, Rodney, J, Guggenheim Fellow, 1986-1987

Bartlett, Rodney, J, Chairman, Subdivision of Theoretical Chemistry, American Chemical Society, August, 1987

Bartlett, Rodney, J, Mulliken Lecturer, University of Georgia, 1993
Bartlett, Rodney, J, Cherry Emerson Lecturer, Emory University, 1992
Bartlett, Rodney J, Fulbright Distinguished Lecturer, Univ. of Arkansas, 1985.