This report summarized publications and invited presentations supported by our AFOSR grant on "Molecular Interactions with Many-Body Methods." In this effort new many-body methods have been developed to treat open-shell molecules; to apply to properties like moments, polarizabilities, hyperpolarizabilities, spin-densities and spin-spin coupling constants; infra-red spectra; and a variety of applications to interesting molecules including the unknown metastable N₂H₅ system. The latter molecule, though isoelectronic with ozone and cyclopropane, is not known experimentally. However, we have predicted its IR spectra to aid in its experimental identification, which should be possible in matrix isolation. Other applications has focused on the accurate, numerical orbital treatment of anions.
I. PUBLICATIONS AND PRESENTATIONS SUPPORTED BY AFOSR (1986-present)


**INVITED PRESENTATIONS (1986 - present)**

<table>
<thead>
<tr>
<th>Month</th>
<th>Year</th>
<th>Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aug.</td>
<td>1988</td>
<td>Sixth International Congress on Quantum Chemistry, Jerusalem, Israel.</td>
</tr>
<tr>
<td>June</td>
<td>1988</td>
<td>Workshop on Quantum Chemistry, Basic Aspects, Actual Trends, Girona, Spain.</td>
</tr>
<tr>
<td>July</td>
<td>1987</td>
<td>American Conference on Theoretical Chemistry, Gull Lake, MN.</td>
</tr>
<tr>
<td>June</td>
<td>1987</td>
<td>The Ninth Annual West Coast Theoretical Chemistry Conference, Berkeley, CA.</td>
</tr>
<tr>
<td>May</td>
<td>1987</td>
<td>Fifth School of Advanced Methods of Quantum Chemistry, &quot;Frontiers of Atomic and Molecular Structure Theory,&quot; Bachotek, Poland.</td>
</tr>
<tr>
<td>April</td>
<td>1987</td>
<td>National ACS Meeting, Symposium on Applications of New Methods for Correlated Ab Initio Studies of Large Molecules, Denver, CO.</td>
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</tbody>
</table>
April 1987 National APS Meeting, Division of Atomic Molecular and Optical Physics, Symposium on Many-Body Physics, Crystal City, VA.
March 1987 Parr/Eliel Symposium, Chapel Hill, NC.
June 1986 Canadian Symposium on Theoretical Chemistry, Toronto, Ontario, Canada
April 1986 Workshop on Interface between Electronic Structure and Dynamics, Snowbird, Utah.

III. Non-refereed Papers - None

IV. Honors

Rodney J. Bartlett has been promoted from Professor to Graduate Research Professor of Chemistry and Physics. The latter rank, which is the highest offered by the University of Florida, is held by only 2% of the faculty.

Three of Dr. Bartlett's papers (published 1978-1981) and supported by AFOSR have recently been designated as Science Citations Classics. Classics are determined by frequency of citation by other scientists and must be among the most cited papers in their respective journals. His paper in Physica Scripta 21, 255 (1980), "Molecular Applications of Coupled-Cluster and Many-Body Perturbation Methods," in the Proceedings of Nobel Symposium Issue, is the third most cited paper in the history of that journal, being cited over 160 times. His paper from the International Journal of Quantum Chemistry 14, 561 (1978), "Many-Body Perturbation Theory, Coupled Pair Many Electron Theory, and the Importance of Quadruple Excitations for the Correlation Problem," has been cited over 200 times, and is the eighth most cited paper in that journal's history. His review in Annual reviews of Physical Chemistry 32, 359 (1981), "Studies of Electron Correlation in Molecules with Many-Body Perturbation Theory and Coupled Cluster Methods," has also been cited over 200 times, and is the twelfth most cited paper in that review series.

V. Patent Requests - None

VI. Patents Granted - None

VII. Students Supported by Grant

D. Bernholdt
D. Magers
S. Zarrabian
E.A. Salter
G. Trucks
T. Pluta
VIII. Postdoctoral Associates Supported by Grant

S. Pal
M. Rittby
G. Fitzgerald
L. Adamowicz
C. Sosa
J. Watts
R.E. Brown (visiting research associate)
S. Kucharski (visiting research associate)

IX. Students Under AFOSR Support Graduated

S. Zarrabian - Convergence to the Solution of the Eigenvalue Problem by Perturbative Methods (December, 1987)
