Dr. Rodney J. Bartlett

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DOB: March 31, 1944, Memphis, TN

Education and Fellowships

B.S., Double Major, Chemistry and Mathematics, Millsaps College, 1966
Ph.D., Quantum Chemistry, University of Florida, Quantum Theory Project, 1971
NSF Postdoctoral Fellow, Aarhus University, Aarhus, Denmark, 1971-1972
Postdoctoral Research Associate, the Johns Hopkins University, 1972-1974
Guggenheim Fellow, Harvard, 1986, Berkeley, 1987.
E.T.S. Walton Fellow, University College and Tyndall Research Institute, Cork, Ireland, 2003.

Research

Rod Bartlett pioneered the development of coupled-cluster (CC) theory and its equation-of-motion EOM-CC extensions to offer highly accurate solutions of the Schrödinger equation for molecular structure and spectra. His group is responsible for the widely used ACES II and III program systems Other research topics include the search for metastable, high-energy density molecules like N_5^-, tetrahedral N_4, and N_8 which he predicted to exist, and provided quantitative spectroscopic fingerprints for their identification. N_5^- and N_5O^+ have been seen in mass spectroscopy. N_8 was recently trapped in a nanotube. His work on non-linear optics and NMR spin-spin coupling constants were the first to provide predictive quality theoretical values for such quantities, enabling the resolution of discrepancies between theory and experiment and predictions in their absence. Recent work includes high-quality electronic spectra of nucleic acid bases in various environments. In other theory his group introduced the natural linear scaled CC method (NLSCC) for very large molecules that builds the observed transferability of chemistry into the theory. They have also introduced new correlated quantum chemical methods for polymers; '*ab initio* density functional theory;' the 'transfer Hamiltonian" for large scale quantum mechanical simulations of materials, and are currently inventing new correlated orbital theories to provide accurate results for large molecules inexpensively, while providing a conceptually attractive molecular orbital interpretation of I and A correlated orbitals whose eigenvalues have to correspond to exact principal IP's and EA's.

Awards and Honors

The American Chemical Society (ACS) award in Theoretical Chemistry (2007)
The Schrödinger Medal of the World Association of Theoretical and Computational Chemists (WATOC) (2008)
The Boys-Rahman Prize of the Royal Society of Chemistry (RSC) (2009)
The Southern Chemist of the Year (2010), Memphis section of the ACS

Humboldt Senior Research Award (2014)
The Florida ACS Award (2000)
Doctor of Science, Honoris Causa, Comenius University, Bratislava, Slovakia October, 2012
Doctor of Science, Honoris Causa, Millsaps College, April, 2011

Memberships

Professor Bartlett is a fellow of the International Academy of Quantum Molecular Sciences (1991), the American Physical Society (1986), the Guggenheim Foundation (1986), and the American Chemical Society (2010). He served as chairman of the Subdivision of Theoretical Chemistry of the ACS (1987). He serves on the advisory boards of the New Zealand Institute of Advanced Study and the Tyndall Research Institute, Cork, Ireland.

Professional Experience

After postdoctoral work, Dr. Bartlett spent 7 years at Battelle Memorial Institute, first at the DOE's Pacific Northwest (National) Laboratory and then at Battelle in Columbus, Ohio. In 1981 he moved to the University of Florida as Professor of Chemistry and Physics, associated with the Quantum Theory Project. He was named Graduate Research Professor in 1987, a rank held by only a handful of faculty. He is the director of the Quantum Theory Project. He maintains a group of a dozen people. He has published over 520 papers and 39 book chapters, presented over 200 invited lectures at major meetings, edited six books, and co-authored an advanced text on many-body methods. He has served on the editorial boards of the Journal of Chemical Physics, Molecular Physics, International Journal of Quantum Chemistry, and Theoretical Chemistry Accounts. He is the principal organizer of the Sanibel meetings, now in their 55th year, and has also organized a number of other meetings for the ACS and other organizations. He was honored by the 7th Molecular Quantum Mechanics meeting, in Lugano, CH, June 2013, Proceedings, Molecular Physics, **112,** Nos. 5-6 (2014) . A meeting on the "Systematic Treatment of Electron Correlation: A Celebration of the Science of Rodney J. Bartlett," was held in April, 2004, St. Simon's Island, Georgia, USA. The Proceedings for the latter is in Molecular Physics, **103**, Nos. 15-16 (2005).

Dr. Bartlett's H-index is 98 (Web of Science) and 106 (Google Scholar). His Researcher ID is F-6781-2011.

Representative Publications

R. J. Bartlett and M. Musial, "Coupled-cluster theory in quantum chemistry", Revs. Modern Phys. **79,** 291-352 (2007).

R. J. Bartlett, "Towards an exact correlated orbital theory for electrons," Frontiers Article, Chem. Phys. Lett. **484**, 1-9 (2009).

I. Shavitt and R.J. Bartlett, "Many-Body Methods in Chemistry and Physics: MBPT and Coupled-Cluster Theory*,* "Cambridge University Press, pp. 1-532 (2009)

Special Invited Lectureships

October 2013 – Lise Meitner Lectures, Weisman Institute of Science, Rehovoth, Israel
January 2013 - Ernest Davidson Lecture, North Texas State University, Dallas, Texas
November 2010 - Russell Pitzer Lecture, Ohio State University, Columbus, Ohio
June 2009 – Per-Olöv Löwdin Lecture, Uppsala University, Uppsala, Sweden