

Rodney J. Bartlett

Graduate Research Professor, Chemistry and Physics, Quantum Theory Project

Professional Preparation

Milsaps College	chemistry and mathematics	B.S., 1966
University of Florida	theoret. chem. physics	Ph.D., 1971
Aarhus Univ., Denmark	theoret. chem. physics	1971-72
	NSF Postdoctoral Fellow	
Johns Hopkins Univ.	theoret. chem. physics	1973-74

Appointments

1988–present	Grad. Research Prof., Chemistry and Physics	Univ. Florida
1981–87	Prof., Chemistry and Physics	Univ. Florida
1979–81	Group Leader, Chem. Physics,	Battelle Mem. Inst.
1977–79	Senior Res. Scientist	Battelle Mem. Inst.
1976–77	Senior Res. Scientist	Battelle Pacific N.W. Lab.
1975-77	Adj. Asst. Prof.	Joint Center Graduate Study Washington State University
1974–76	Principal Res. Scientist	Battelle Pacific N.W. Lab.

Publications Related to the Project 480 refereed papers and book chapters. Senior copyright holder for the ACES II and III Program Systems

- R. J. Bartlett, “Electron Correlation from Molecules to Materials,” in *Electron Correlations and Materials Properties 2* (T. Gonis, N. Kioussis and M. Ciftan, editors), Kluwer Academic, Plenum Publishers, 219-236 (2003). RJB., Invited paper, Second International Workshop on Electron Correlations in Solids and Materials, Rhodes, Greece.
- Y.W. Hsiao, K. Runge, M.G. Cory and R.J. Bartlett, “Direct Molecular Dynamics Using Quantum Chemical Hamiltonians: C60 Impact on a Passive Surface”, *J. Phys. Chem.* **105**, 7004-7010 (2001).
- C.E. Taylor, M.G. Cory, R.J. Bartlett and W. Thiel, “The transfer Hamiltonian: a tool for large scale simulations with quantum mechanical forces, “ *Comp. Mater. Sci.* **27**, 204-211 (2003); Part of RJB Invited Paper at European M.R.S., Strasbourg, France.
- J. McClellan, T. Hughes and R.J. Bartlett, “Applications of the transfer Hamiltonian formalism to high energy model systems,” *Int. J. Quantum Chem, Symp.* **105**, 914 (2005).
- A. Korkin, J.C. Greer, G. Bersuker, V. Karasiev, and R.J. Bartlett, “Computational Design of Si/SiO₂ interfaces: Stress and strain on the atomic scale,” *Phys. Rev. B* **73**, 165312 (2006).

Other Significant Publications

- R. J. Bartlett, V. F. Lotrich, I.V. Schweigert, “Ab initio DFT: The best of both worlds?” *J. Chem. Phys.* **123**, 062205 (2005).
- R. J. Bartlett and G. D. Purvis, “Many-body perturbation theory, coupled-pair many-electron theory and the importance of quadruple excitations for the correlation problem,” *Proceedings of the American Theoretical Chemistry Conference, Boulder, Colorado, Int. J. Quantum Chem.* **14**, 561-581 (1978).
- R.J. Bartlett, “Many-body perturbation theory and coupled cluster theory for electron correlation in molecules,” *Ann. Rev. Phys. Chem.* **32**, 359- (1981).
- G. D. Purvis, III and R. J. Bartlett, “A full coupled-cluster singles and doubles model: The inclusion of disconnected triples,” *J. Chem. Phys.* **76**, 1910-1918 (1982).
- R. J. Bartlett, “Coupled-cluster approach to molecular structure and spectra: A step toward predictive quantum chemistry”, *J. Phys. Chem.* **93**, 1697-1708 (1989) (Feature Article)

Synergistic Activities

- American Chemical Society Award in Theoretical Chemistry, 2007.
- Schrödinger Medal, WATOC, 2008.
- Florida Award, 2000.
- Guggenheim Fellow, Harvard University, University of California at Berkeley, 1986–1987.
- Fellow, American Physical Society, 1989
- Fellow, International Academy of Quantum Molecular Sciences, 1991
- Editorial Boards, *Theoretical Chemistry Accounts* (1997-present); *Molecular Physics* (1999-present)

Collaborators and Other Affiliations Collaborators: A. Al-Derzi (U. Florida), S. Trickey (U. Florida), S. Yip (MIT), F. Harris (U. Florida), S. Kucharski (Katowice), W. Thiel (Max Plank), A. Perera (U. Florida), J. Lee (Korea), Chantal Daniel (Strasbourg), Jim Greer (Tyndale Institute, Cork, Ireland), J. Del Bene (Youngtown State, Ohio), Garnet Chan (Cornell).

Ph.D. advisors were: P-O. Löwdin (deceased) and N.Yngve Öhrn

Postdoctoral mentors were: R.G. Parr (Johns Hopkins, now Univ. N. Carolina), J. Lindenberg (Aarhus Univ., Denmark)

Ph.D Students supervised: Denis Bokhan (2007), Igor Schweigert (2005), Ariana Beste (2004), Tom Henderson, (2004). Carlos Taylor (2004), Motoi Tobita (2002), Ken Wilson (2002), Rene Peloquin-Mattie(1999), Piotr Rozyczko(1998), Steve Gwaltney(1997), Jun Sun(1997), Ajith Perera(1994), David Bernholdt(1993), Walt Lauderdale(1991), Tadeus Pluta(1990), Gary Trucks(1988), Alan Salter(1988), David Magers(1988), Sohrab Zarrabian(1987).

Postdoctorals (2005-present): Osama Hino, Norbert Flocke, Keith Runge, Marshall Cory, Monica Musial, So Hirata, Ireneuze Grabowski, Victor Lotrich, Takahashi Tsuchiya, Tomas Kus, Afaf Al-Derzi, Stefan Fau, Tomoko Kinoshita.