

## Ron Shepard

Argonne National Laboratory  
Chemical Sciences and Engineering Division  
9700 South Cass Avenue, Building 200  
Argonne, IL 60439-4837  
phone: 630/252-3584, fax: 630/252-9292  
e-mail: shepard@tcg.anl.gov

### Professional Experience

- **2007-present.** Senior Scientist, Chemical Sciences and Engineering Division, Argonne National Laboratory.
- **1986-2007.** Scientist, Chemistry Division, Argonne National Laboratory.
- **1981-1986.** Assistant Scientist, Chemistry Division, Argonne National Laboratory.
- **January 1981-October 1981.** Research Scientist, Battelle Columbus Laboratories, Columbus, Ohio.
- **1980-1981.** Postdoctoral Appointment, Battelle Columbus Laboratories, Columbus, Ohio. Battelle Technical Development Post Doctoral Fellowship. (Advisor: Professor I. Shavitt).

### Education

- Ph.D., Physical Chemistry, University of Utah, 1980. Calhoun-Halkjaer Award for Outstanding Research (1979). (Advisor: Professor J. Simons).
- B.S., Mathematics and Chemistry, University of Central Arkansas, 1975. Trinity Foundation Scholar (1970-1975). (Advisor: Professor J. M. Manion).

### Awards

- Argonne Laboratory Director's Award (2007)
- Argonne Pacesetter Award (2006)

### Career Activities & Highlights

- Areas of Research and Expertise
  - This project involves the development, implementation, and application of theoretical methods for the calculation and characterization of potential energy surfaces involving molecular species that occur in hydrocarbon combustion. The methods that are developed in this project advance the state of the art by exploiting new technology, including parallel computers.
- Professional Organizations

- Editor, *Chemical Physics* (special editor, 2006-2007)
- American Chemical Society, Division of Physical Chemistry
- Sigma Xi, The Scientific Research Society
- Gaussian Scientific Advisory Board (1993-1997)
- American Association for the Advancement of Science
  
- Outside Collaborations
  - J.-P. Blaudeau (Wright-Patterson AFB)
  - S. R. Brozell (Ohio Supercomputer Center)
  - M. Dvorak (MCS-ANL)
  - G. Kedziora (Wright-Patterson AFB)
  - H. Lischka (University of Vienna, Austria)
  - T. Muller (Julich Research Center, Germany)
  - M. Minkoff (CHM-ANL)
  - J. T. Muckerman (Brookhaven National Laboratory)
  - R. M. Pitzer (Ohio State University)
  - M. Seth (University of Calgary, Canada)
  - I. Shavitt (University of Illinois)
  - E. A. Stahlberg (Ohio Supercomputer Center)
  - P. G. Szalay (Etvos Lorand University, Hungary)
  - D. R. Yarkony (Johns Hopkins University)
  - Z. Zhang (Stanford University)

## Publications

Edited by M. Barbatti, H. Köppel, R. Shepard, and P. G. Szalay, "Electron Correlation and Molecular Dynamics for Excited States and Photochemistry," Special Issue in Honor of Hans Lischka, *Journal of Chemical Physics*, 349(1-3), (2008).

R. Shepard, "Advanced Software for the Calculation of Thermochemistry, Kinetics, and Dynamics," *Journal of Physics*, Conf. Series 125, 012016 (2008).

R. Shepard, G. S. Kedziora, H. Lischka, I. Shavitt, T. Müller, P. G. Szalay, M. Kállay, M. Seth, "The Accuracy of Molecular Bond Lengths Computed by Multireference Electronic Structure Methods," *Journal of Chemical Physics*, 349, 37-57 (2008).

R. Shepard and M. Minkoff, "Some Comments on the DIIS Method," *Molecular Physics*, 105, 2839-2848 (2007).

S. R. Brozell, R. Shepard, and Z. Zhang, "Spin-Orbit Interaction with Nonlinear Wave Functions," *International Journal of Quantum Chemistry*, 107, 3191-3202 (2007).

R. Shepard, M. Minkoff, and S. R. Brozell, "Nonlinear Wave Function Expansions: A Progress Report," *International Journal of Quantum Chemistry*, 107, 3203-3218 (2007).

R. Shepard, "Advanced Software for the Calculation of Thermochemistry, Kinetics, and Dynamics," *Journal of Physics*, Conf. Series 78, 012067 (2007).

R. Shepard and M. Minkoff, "Optimization of Nonlinear Wave Function Parameters," *International Journal of Quantum Chemistry*, 106 (15), 3190-3207 (2006).

R. Shepard, "Hamiltonian Matrix and Reduced Density Matrix Construction with Nonlinear Wave Functions," *The Journal of Physical Chemistry*, 110 (28), 8880-8892 (2006).

R. Shepard, "A General Nonlinear Expansion Form for Electronic Wave Functions," *The Journal of Physical Chemistry, A* 109 (50), 11629-11641 (2005).

Y. Zhou, R. Shepard, and M. Minkoff, "Computing Eigenvalue Bounds for Iterative Subspace Matrix Methods," *Computer Physics Communications Package*, 167 (2), 90-102 (2005).

R. Shepard, M. Minkoff, and Y. Zhou, "Software for Computing Eigenvalue Bounds for Iterative Subspace Matrix Methods," *Computer Physics Communications Package*, 170 (1), 109-114 (2005).