

Lawrence B. Harding

Argonne National Laboratory
Chemical Sciences and Engineering Division
9700 South Cass Avenue, Building 200
Argonne, IL 60439-4837
phone: 630/252-3591, fax: 630/252-9292
e-mail: harding@anl.gov

Professional Experience

- **2007-Present.** Argonne Distinguished Fellow, Chemical Sciences and Engineering Division.
- **1998-2007.** Senior Scientist, Chemistry Division, Argonne National Laboratory.
- **1984-1998.** Scientist, Chemistry Division, Argonne National Laboratory.
- **1992-1993.** Visiting Fellow, Joint Institute for Laboratory Astrophysics, Boulder, Colorado.
- **1979-1984.** Assistant Scientist, Chemistry Division, Argonne National Laboratory.
- **1978-1979.** National Science Foundation National Needs Fellow, Carnegie-Mellon University.

Education

- Ph.D., Chemistry, California Institute of Technology, 1979. (Advisor: W. A. Goddard III)
- B.A., Chemistry and Mathematics, Wesleyan University, 1973.

Awards

- Fellow, American Association for the Advancement of Science (2006)
- University of Chicago Distinguished Performance Award (2004)
- Argonne Pacesetter Award (2002)
- Herbert Newby McKoy Award (1978)
- Graham Prize in the Natural Sciences (1973)

Career Activities & Highlights

- Areas of Research and Expertise
 - Applications of *ab initio* electronic structure theory to reactive and non-reactive potential energy surfaces.
- Professional Organizations
 - Phi Beta Kappa
 - American Chemical Society
 - Combustion Institute
 - American Association for the Advancement of Science

- Outside Collaborations
 - J. M. Bowman (Emory University)
 - S. Carter (Emory University)
 - R. J. Cody (NASA/Goddard Space Flight Center)
 - Y. Georgievskii (Sandia National Laboratory)
 - A. A. Golubeva (University of Southern California)
 - Y. Guo (University of Missouri-Columbia)
 - K. S. Gupte (University of Illinois, Chicago)
 - X. Huang (Emory University)
 - A. W. Jasper (Sandia National Laboratory)
 - A. I. Krylov (University of Southern California)
 - J. A. Miller (Sandia National Laboratory)
 - F. L. Nesbitt (NASA/Goddard Space Flight Center)
 - J. K. Parker (NASA/Goddard Space Flight Center)
 - W. A. Payne (NASA/Goddard Space Flight Center)
 - A. V. Nemukhin (University of Southern California)
 - L. J. Stief (NASA/Goddard Space Flight Center)
 - D. L. Thompson (University of Missouri-Columbia)
 - X. Zhang (Emory University)

Publications

L. B. Harding, S. J. Klippenstein, and J. A. Miller, "The Kinetics of Ch + N₂ Revisited with Multireference Methods," *The Journal of Physical Chemistry, A* 112, 522-532 (2008).

L. B. Harding, S. J. Klippenstein, and A. W. Jasper, "AB *Initio* Methods for Reactive Potential Surfaces," *Physical Chemistry Chemical Physics*, 9 (31), 4055-4070 (2007).

H. Fan, L. B. Harding, and S. T. Pratt, "Dissociative Ionization of Hot C₃h₅ Radicals," *Molecular Physics*, 105, 1517-1534(2007).

A. W. Jasper, S. J. Klippenstein, L. B. Harding, and B. Ruscic, "Kinetics of the Reaction of Methyl Radical with Hydroxyl Radical and Methanol Decomposition," *The Journal of Physical Chemistry, A* 111 (19), 3932-3950 (2007).

L. B. Harding, S. J. Klippenstein, and Y. Georgievskii, "On the Combination Reactions of Hydrogen Atoms with Resonance Stabilized Hydrocarbon Radicals," *The Journal of Physical Chemistry, A* 111 (19), 3789-3801 (2007).

K. S. Gupte, J. H. Kiefer, R. S. Tranter, S. J. Klippenstein, and L. B. Harding, "Decomposition of Acetaldehyde: Experiment and Detailed Theory," *Proceedings of the Combustion Institute*, 31 (1), 167-174 (2007).

S. J. Klippenstein, L. B. Harding, and Y. Georgievskii, "On the Formation and Decomposition of C₇H₈," *Proceedings of the Combustion Institute*, 31 (1), 221-229 (2007).

S. J. Klippenstein, Y. Georgievskii, and L. B. Harding, "Predictive Theory for the Association Kinetics of Two Alkyl Radicals," *Physical Chemistry Chemical Physics* 8 (10), 1133-1147 (2006).

D. M. Medvedev, L. B. Harding, and S. K. Gray, "Methyl Radical: Ab Initio Global Potential Surface, Vibrational Levels, and Partition Function," *Molecular Physics*, 104 (1), 73-81 (2006).

L. B. Harding, Y. Georgievskii, and S. J. Klippenstein, "Predictive Theory for Hydrogen Atom – Hydrocarbon Radical Association Kinetics," *The Journal of Physical Chemistry, A* 109 (21), 4646-4656 (2005).

L. B. Harding, S. J. Klippenstein, and Y. Georgievskii, "Reactions of Oxygen Atoms with Hydrocarbon Radicals: A Priori Kinetic Predictions for the CH₃ + O, C₂H₅ + O, and C₂H₃ + O Reactions," *Proceedings of the Combustion Institute*, 30, 985-993 (2005).