

CURRICULUM VITAE

Ronald J. Duchovic
Department of Chemistry
Indiana University Purdue University Fort Wayne
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Fort Wayne, IN 46805-1499
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Education

Sabbatical Leave:

Argonne National Laboratory, 8-99 to 12-99
Theoretical Chemistry Group: Albert F. Wagner

Postdoctoral Fellowship:

Argonne National Laboratory, 2-86 to 12-87
Theoretical Chemistry Group: Thomas H. Dunning

Northwestern University, 1-84 to 6-85
Research Director: George C. Schatz

Ph.D. (Physical Chemistry, Theoretical), Wayne State University, 1984

Thesis: Studies in Molecular Dynamics: The $\text{CH}_4 \leftrightarrow \text{CH}_3 + \text{H}$ Potential Energy Surface and Semiclassical Eigenvalues of a Model Alkyl Radical
Adviser: William L. Hase

M.S. (Mathematics), University of Michigan, 1975

B.S. (Mathematics), University of Notre Dame, 1973

Grants

National Science Foundation, 12 month project extension, August, 2007 – August, 2008
Conference Stipend, Chair's Fund, Gordon Research Conference, July, 2006
IPFW LEAD Grant, 2005 (Co-PIs: R. M. Berger, M. R. Columbia, A. W. Friedel)
National Science Foundation, September, 2004 – August, 2007
IPFW Overseas Conference Fund travel grant, August, 2004
Indiana University Overseas Conference Fund travel grant, May, 2004
Research Contract, Argonne National Laboratory, June, 2002 – June, 2003
Conference Stipend, Chair's Fund, Gordon Research Conference, July, 2002
Argonne National Laboratory, Sabbatical Leave, August – December, 2000
Grant of 10 000 SU hours, NCSA, 2000 – 2001

Research Contract, Argonne National Laboratory, June – August, 2000
Argonne National Laboratory, Sabbatical Leave, August – December, 1999
Visiting Research Scientist, Argonne National Laboratory, June – August, 1999
Purdue Research Foundation Faculty Summer Grant, 1997
Grant of instructional CPU time, San Diego Supercomputer Center, 1997
American Chemical Society, Petroleum Research Fund, Type B, 1997 – 1999
IPFW Faculty Summer Grant, 1994
American Chemical Society, Petroleum Research Fund, Type B, 1994 – 1996
American Chemical Society, Petroleum Research Fund, Type GB, 1992 – 1994
Grant of instructional CPU time, San Diego Supercomputer Center, 1992
IPFW Faculty Summer Grant, 1991
GOAP Grant, 1991

Publications

R. J. Duchovic and Joel A. Vilensky, “Mustard Gas: Its Pre-World War I History”, *J. Chem. Ed.*, **84**, 944(2007).

R. J. Duchovic, “Connecting Scholarship and Social Responsibility”, in *Quick Hits for Educating Citizens*, edited by James L. Perry and Steven G. Jones, Indiana University Press, 2006.

R. J. Duchovic and Marla A. Parker, “A Quasi-Classical Trajectory Study of the Reaction $H + O_2 \rightleftharpoons OH + O$ with the O_2 Reagent Vibrationally Excited”, *J. Phys. Chem. A*, **109**, 5883(2005).

R. J. Duchovic, Y. L. Volobuev, G. C. Lynch, D. G. Truhlar, T. C. Allison, A. F. Wagner, B. C. Garrett, and J. Corchado, “Erratum: POTLIB 2001: A Potential Energy Surface Library for Chemical Systems” , [*Computer Physics Communications*, **144** (2002) 169-187], *Computer Phys. Comm.*, **156**, 319(2004).

R. J. Duchovic, Y. L. Volobuev, G. C. Lynch, D. G. Truhlar, T. C. Allison, A. F. Wagner, B. C. Garrett, and J. Corchado, “POTLIB 2001: A Potential Energy Surface Library for Chemical Systems”, *Computer Phys. Comm.*, **144**, 169(2002).

R. J. Duchovic, “Teaching College General Chemistry: Techniques Designed to Communicate a Conceptual Framework”, *JCE Online.*,
<http://jchemed.chem.wisc.edu/Journal/Issues/1998/Jul/abs856.html>.

R. J. Duchovic, “Teaching College General Chemistry: Techniques Designed to Communicate a Conceptual Framework”, *J. Chem. Educ.*, **75**, 856(1998).

R. J. Duchovic, D. P. Maloney, A. Majumdar, and R. S. Manalis, “Teaching Science to the Non-Science Major: An Interdisciplinary Approach”, *Journal of College Science Teaching*, **XXVII**, 258(1998).

- W. L. Hase, R. J. Duchovic, X. Hu, A. Komornicki, K. F. Lim, D-h. Lu, G. H. Peslherbe, K. N. Swamy, S. R. Vande Linde, A. J. C. Varandas, H. Wang, and R. J. Wolf, VENUS96: A General Chemical Dynamics Computer Program”, *QCPE Bull*, **16**, 43(1996).
- R. J. Duchovic, J. D. Pettigrew, B. Welling, and T. Shipchandler, “Conventional Transition State Theory/Rice-Ramsperger-Kassel-Marcus Theory Calculations of Thermal Termolecular Rate Coefficients for $\text{H(D)} + \text{O}_2 + \text{M}$ ”, *J. Chem. Phys.*, **105**, 10367(1996).
- R. J. Duchovic and J. D. Pettigrew, “An Application of Conventional Transition State Theory To Compute High-Pressure Limit Thermal Rate Coefficients for the Reaction: $\text{H(D)} + \text{O}_2 \rightleftharpoons \text{H(D)O}_2^* \rightleftharpoons \text{OH(D)} + \text{O}$ ”, *J. Phys. Chem.*, **98**, 10794(1994).
- S. P. Walch and R. J. Duchovic, “Erratum: Theoretical Characterization of the Potential Energy Surface for $\text{H} + \text{O}_2 \rightleftharpoons \text{HO}_2^* \rightleftharpoons \text{OH} + \text{O}$. III. Computed Points to Define a Global Potential Energy Surface”, [*J. Chem. Phys.*, **94**, 7068(1991)], *J. Chem. Phys.*, **96**, 4050(1992).
- S. P. Walch and R. J. Duchovic, “Theoretical Characterization of the Potential Energy Surface for $\text{H} + \text{O}_2 \rightleftharpoons \text{HO}_2^* \rightleftharpoons \text{OH} + \text{O}$. III. Computed Points to Define a Global Potential Energy Surface”, *J. Chem. Phys.*, **94**, 7068(1991).
- R. J. Duchovic, A. F. Wagner, R. E. Turner, D. M. Garner, and D. G. Fleming, “The Analysis of Muonium Hyperfine Interaction Measurements of Thermal Rate Constants for Addition Reactions”, *J. Chem. Phys.*, **94**, 2794(1991).
- S. P. Walch, R. J. Duchovic, and C. M. Rohlfing, “Theoretical Characterization of the Minimum Energy Path for Hydrogen Atom Addition to N_2 : Implications for the Unimolecular Lifetime of HN_2 ”, *J. Chem. Phys.*, **90**, 3230(1989).
- W. L. Hase, S. L. Mondro, R. J. Duchovic, and D. M. Hirst, “Thermal Rate Constants for $\text{H} + \text{CH}_3 \rightarrow \text{CH}_4$ Recombination. II. Comparison of Experiment and Canonical Variational Transition State Theory”, *J. Am. Chem. Soc.*, **109**, 2916(1987).
- R. J. Duchovic and G. C. Schatz, “The FFT Method for Determining Semiclassical Eigenvalues: Application to Asymmetric Top Rigid Rotors”, *J. Chem. Phys.*, **84**, 2239(1986).
- W. L. Hase and R. J. Duchovic, “Thermal Rate Constant for $\text{H} + \text{CH}_3 \rightarrow \text{CH}_4$ Recombination. Comparison of Quasiclassical Trajectory and Variational Transition State Theory”, *J. Chem. Phys.*, **83**, 3448(1985).
- R. J. Duchovic and W. L. Hase, “A Dynamical Study of the $\text{H} + \text{CH}_3 \rightarrow \text{CH}_4$ Recombination Reaction”, *J. Chem. Phys.*, **82**, 3599(1985).
- R. J. Duchovic and W. L. Hase, “Sensitivity of the $\text{H} + \text{CH}_3 \rightarrow \text{CH}_4$ Recombination Rate Constant to the Shape of the CH Stretching Potential”, *Chem. Phys. Lett.*, **110**, 474(1984).

R. J. Duchovic, K. N. Swamy, and W. L. Hase, "Semiclassical Vibrational Eigenvalues of a Three-Dimensional Hamiltonian", *J. Chem. Phys.*, **80**, 1462(1984).

W. L. Hase, R. J. Duchovic, K. N. Swamy, and R. J. Wolf, "Trajectory Studies of Model $\text{HCC} \rightarrow \text{H} + \text{C} = \text{C}$ Dissociation. III. Details of the Lifetime Distribution Following Chemical Activation", *J. Chem. Phys.*, **80**, 714(1984).

R. J. Duchovic, W. L. Hase, and H. B. Schlegel, "Analytic Function for the $\text{H} + \text{CH}_3 \leftrightarrow \text{CH}_4$ Potential Energy Surface", *J. Phys. Chem.*, **88**, 1339(1984).

R. J. Duchovic, W. L. Hase, H. B. Schlegel, M. J. Frisch, and K. Raghavachari, "Ab Initio Potential Energy Curve for CH Bond Dissociation in Methane", *Chem. Phys. Lett.*, **89**, 120(1982).

Conference Participation

XXIst Conference on the Dynamics of Molecular Collisions, La Fonda Hotel,
Santa Fe, NM, July, 2007.
Poster Presentation

FACET (Faculty Colloquium on Excellence in Teaching) Retreat IUPUI, IN May 18 – 19,
2007.
Conferee, FACET Steering Committee member (IPFW Representative)

19th Biennial Conference on Chemical Education (BCCE) Purdue University, West
Lafayette, IN, July, 2006
Conferee

Gordon Research Conference: Atomic and Molecular Interactions, Colby–Sawyer College,
New London, New Hampshire, July, 2006
Poster Presentation

National Computational Science Institute
2006 Workshops for Undergraduate Faculty: Parallel Computing at Houston Community
College
May 21 – May 26, 2006

FACET (Faculty Colloquium on Excellence in Teaching) Retreat Potawatomi Inn, Pokagon
State Park, IN May 19 – 21, 2006.
Conferee, FACET Steering Committee member (IPFW Representative)

XXth Conference on the Dynamics of Molecular Collisions, Asilomar Conference Center,
Pacific Grove, CA, July, 2005
Poster Presentation

FACET (Faculty Colloquium on Excellence in Teaching) Retreat Potawatomi Inn, Pokagon State Park, IN May 20 – 22, 2005.

Member of Retreat Planning Committee

Oral Presentation: “Symmetry: The Song of the Universe”

18th International Symposium on Gas Kinetics, University of Bristol, Bristol, United Kingdom, August, 2004

Poster Presentation

XIXth Conference on the Dynamics of Molecular Collisions, Granlibakken Resort, Lake Tahoe, CA, July, 2003

Poster Presentation

FACET (Faculty Colloquium on Excellence in Teaching) Retreat Fourwinds Resort and Marina, Bloomington, IN May 16 –18, 2003.

New FACET Inductee, Class of 2003

Gordon Research Conference: Atomic and Molecular Interactions, Roger Williams University, Bristol, Rhode Island, July, 2002.

Poster Presentation

Thirty-fourth Annual Midwest Theoretical Chemistry Conference, University of Minnesota, Minneapolis, MN, October, 2001

Poster Presentation

Gordon Research Conference: Atomic and Molecular Interactions, Colby–Sawyer College, New London, New Hampshire, July, 2000.

Poster Presentation

Assessment 2000 Conference, American Association for Higher Education, Charlotte, NC, June, 2000

Representative of IPFW

1999 Conference on the Dynamics of Molecular Collisions, Splitrock Resort, New Harmony, PA, July, 1999

Poster Presentation

Thirty-Second Annual Midwest Theoretical Chemistry Conference, University of Notre Dame, Notre Dame, IN, May, 1999

Poster Presentation

Lilly Endowment – Retention Initiatives: Year One Capstone Conference Purdue University, West Lafayette, IN, September 28, 1998.

Representative of IPFW

Gordon Research Conference: Atomic and Molecular Interactions, Colby–Sawyer College, New London, New Hampshire, July, 1998.

Poster Presentation

The Use of Computers and Related Technologies for Instruction Conference, Ivy Tech State College, Fort Wayne, IN, May 28, 1998.

Oral Presentation

Second Annual FACET Associate Faculty Conference

Conference at IUPUI, October 17 – 18, 1997.

Representative of IPFW

1997 Conference on the Dynamics of Molecular Collisions, Brainerd, MN, July, 1997.

Poster Presentation

IAS (Indiana Institute for Advanced Study) Faculty Forum on Science Funding, Conference at IUPUI, February 24, 1997.

Conferee

“The Future of Technological Education: Developing Appropriate Engineering, Mathematics, and Science Curriculum for the 21st Century”, One–day Conference at the Rose–Hulman Institute of Technology, Terre Haute, IN, August 30, 1996.

Conferee

Supplemental Instruction Supervisor Training Workshop, University of Missouri, Kansas City, MO, July 14 – 17, 1996

Trainee

Gordon Research Conference: Atomic and Molecular Interactions, Colby–Sawyer College, New London, New Hampshire, July, 1996.

Poster Presentation

1995 Conference on the Dynamics of Molecular Collisions, Asilomar CA, July, 1995

Poster Presentation

The Council on Undergraduate Research: Second April Dialogue, Washington, D. C., March 31 – April 1, 1995.

Conferee

Gordon Research Conference: Atomic and Molecular Interactions, Colby–Sawyer College, New London, New Hampshire, July, 1994.

Poster Presentation

Conference on the Dynamics of Molecular Collisions, Unicoi State Park, GA, June, 1993

Poster Presentation

Conference on the Dynamics of Molecular Collisions, Lake George, NY, July, 1991
Poster Presentation

Twenty-fourth Annual Midwest Theoretical Chemistry Conference, May, 1991
Poster Presentation

West Coast Theoretical Chemistry Conference, Salt Lake City, UT, March, 1990
Poster Presentation

Conference on the Dynamics of Molecular Collisions, Asilomar, CA, July, 1989
Poster Presentation

West Coast Theoretical Chemistry Conference, San Jose, CA, May, 1989
Poster Presentation

American Chemical Society Meeting, Toronto, Spring, 1988
Poster Presentation

American Conference on Theoretical Chemistry, Gull Lake, July, 1987
Poster Presentation

Conference on the Dynamics of Molecular Collisions, Wheeling, July, 1987
Poster Presentation

1987 Spring Technical Meeting, Central State Section, The Combustion Institute, May,
1987
Oral Presentation

Nineteenth Annual Midwest Theoretical Chemistry Conference, May, 1986
Conferee

Eighteenth Annual Midwest Theoretical Chemistry Conference, May, 1985
Poster Presentation

Future Directions for Supercomputer Use in Chemistry, October, 1984
Conferee

Seventeenth Annual Midwest Theoretical Chemistry Conference, May, 1984
Poster Presentation

Conference on the Dynamics of Molecular Collisions, Gull Lake, June, 1983
Poster Presentation

Sixteenth Annual Midwest Theoretical Chemistry Conference, May, 1983
Poster Presentation

American Chemical Society Meeting, Kansas City, Fall, 1982
Poster Presentation

Fifteenth Annual Midwest Theoretical Chemistry Conference, May, 1982
Poster Presentation

American Conference on Theoretical Chemistry, Boulder, June, 1981
Conferee

Fourteenth Annual Midwest Theoretical Chemistry Conference, May, 1981
Conferee

Invited Talks

Indiana Institute of Technology, March, 2007

The University of Toledo, Chemistry Department Seminar, May, 1996

Conference on the Integration of Computers and Related Applications into the Curriculum
at IPFW, March 1 – 2, 1993

IPFW Associate Vice-Chancellor's Seminar on Computing: COMPUTERS IN THE
CLASSROOM,
October 19 and 21, 1992

Indiana University Purdue University Fort Wayne, Department of Mathematics Seminar,
November, 1992

Wayne State University, Physical Chemistry Seminar, October, 1991

Departmental Seminars

Indiana University Purdue University Fort Wayne, Department of Chemistry, February,
2004.

Indiana University Purdue University Fort Wayne, Department of Chemistry, February,
2000

Indiana University Purdue University Fort Wayne, Department of Chemistry Colloquium,
March, 1999

Indiana University Purdue University Fort Wayne, Department of Chemistry Colloquium,
December, 1997

Indiana University Purdue University Fort Wayne, Department of Chemistry, October, 1997

Indiana University Purdue University Fort Wayne, Department of Chemistry, February, 1995

Indiana University Purdue University Fort Wayne, Department of Chemistry Colloquium, January, 1995

Indiana University Purdue University Fort Wayne, Department of Chemistry Colloquium, November, 1994

Indiana University Purdue University Fort Wayne, Department of Chemistry, December, 1990

Association Memberships

FACET

American Chemical Society

American Physical Society

American Association for the Advancement of Science

The Combustion Institute

Sigma Xi

Phi Lambda Upsilon

Academic Honors and Awards

Distinguished Service to Science Education, 2002

Science Education Foundation of Indiana (SEFI)

Election to FACET Class of 2003

Graduate:

Knoller Fellowship, Department of Chemistry, 1981–1983

University Graduate Fellowship, Wayne State University, 1980–1981

Undergraduate:

Bachelor of Science with High Honors

National Merit Finalist

Chrysler Fund Merit Scholarship

Michigan Higher Education Assistance Authority Scholarship

UAW Local 412 College Scholarship

Professional Experience

Indiana University Purdue University Fort Wayne
7-96 to Present
Associate Professor of Chemistry

Indiana University Purdue University Fort Wayne
8-90 to 6-96
Assistant Professor of Chemistry

Eloret Institute, Sunnyvale, California
12-87 to 7-90
Research Scientist

Eloret Institute is a non-profit research corporation. I worked as the Principal Investigator on a grant from the National Aeronautics and Space Administration. The research for NASA focused on the kinetics and microscopic dynamics of small molecular systems.

Grace Engineering, Inc. Russellville, Arkansas
6-85 to 2-86
Development Chemist (Chief)

In this position I was responsible for the establishment of a Chemical Sciences Department. This task demanded the utilization of many different areas of chemistry, ranging from physical chemistry to environmental chemistry. The position also entailed significant managerial responsibility both in the organization of the Chemical Sciences Department and in the determination of operating policies for the company as a whole.

Wayne State University, Detroit, Michigan
9-79 to 6-80
Teaching Assistant

I participated in the teaching of General Chemistry. This required conducting quiz classes, running laboratories, and grading both homework and examinations.

Chrysler Corporation, Highland Park, Michigan
9-77 to 9-79
Engineering Staff Member

As a member of the Fuel Economy Planning Office, I performed mathematical and computer-assisted analyses of the Corporate fuel economy improvement plan.

National Security Agency, Fort Meade, Maryland
9-76 to 8-77
Analysis Intern

I was part of the NSA Intern Program which was designed to provide in-depth training in a particular specialty as well as broad exposure to the various functions of the agency. My work focused on mathematical and computer-assisted analysis of data.

Chrysler Corporation, Highland Park, Michigan

2-76 to 9-76

Engineering Staff Member

As a member of the Fuel Economy Planning Office, I performed mathematical and computer-assisted analyses of the Corporate fuel economy improvement plan.