Curriculum Vitae

David M. Leitner
Department of Chemistry and Chemical Physics Program
University of Nevada, Reno/216
Reno, Nevada, 89557
Email: dml@unr.edu
Phone: (775) 784-1968
Website: https://leitnergroup.wixsite.com/dmlpage

Education:

1989	The University of Chicago; Ph.D., Physical Chemistry/Chemical Physics; Research advisor: Professor R. S. Berry
1985	Cornell University; B.S. Chemical Engineering; B.A. Chemistry

Academic Faculty Positions:

2025 -	Foundation Professor, University of Nevada, Reno
2023 -	Regents Research Professor, University of Nevada, Reno
2019 -	Reynold C. Fuson Professor of Chemistry, University of Nevada, Reno
2009 -	Professor, University of Nevada, Reno
2005 - 2009	Associate Professor, University of Nevada, Reno
2000 - 2005	Assistant Professor, University of Nevada, Reno

Research Positions:

1998-2000	Research Faculty, Assistant Project Scientist, UC San Diego
1994-1998	Research Associate, U. Illinois at Urbana-Champaign, with Prof. P. G. Wolynes
1991-1994	Research Associate, Universität Heidelberg, with Prof. L. S. Cederbaum
1990	Postdoctoral Research Associate, Brown University, with Prof. J. Doll

Honors and Awards:

2025	University of Nevada, Reno Foundation Professor
2023	Nevada Board of Regents Distinguished Researcher Award
2019	Japan Society for the Promotion of Science (JSPS) Invitational Fellow
2018	Appointed to Editorial Advisory Board of *Journal of Physical Chemistry*
2018	Appointed Director of UNR's Center for Advanced Studies
2017	Elected Fellow of the American Association for the Advancement of Science (AAAS)
2017	Appointed to Editorial Board of *Scientific Reports - Nature*
2016	Elected Member-at-Large, Executive Committee, ACS Division of Physical Chemistry
2015	Appointed to Editorial Advisory Board of *The Journal of Chemical Physics*
2014	External Senior Fellow, Freiburg Institute for Advanced Studies (FRIAS), University of Freiburg, Germany
2014	University of Nevada, Reno Outstanding Researcher Award

2012	Elected Fellow of the American Physical Society (APS)
2012	Fellow of the International Faculty of the Solvation Science Cluster of Excellence (RESOLV), Ruhr-Universität Bochum
2011	Hyung K. Shin Award for Excellence in Research, U. Nevada, Reno
2010	Elected Secretary/Treasurer of the APS Division of Chemical Physics
2004	Mousel-Feltner Award for Excellence in Research and Creative Activity, University of Nevada, Reno
2001	Research Corporation Research Innovation Award
2000	Camille and Henry Dreyfus New Faculty Award
1999	United Nations International Short Term Advisory Resources Consultant, Department of Physics, Bilkent University, Turkey
1993-1994	Alexander von Humboldt Fellowship
1991-1993	National Science Foundation Postdoctoral Fellowship

Guest Professor:

2019 – 2020 (4 months)	Nagoya University, Japan
2015 (May – July)	Freiburg Institute for Advanced Studies (FRIAS), Germany
2014 (May – Aug.)	Freiburg Institute for Advanced Studies (FRIAS), Germany
2013 (May – July)	Department of Chemistry, Ruhr Universität Bochum
2012 (Jan. – June)	Department of Chemistry, Boston University
2010 (May - July)	Department of Chemistry, Ruhr Universität Bochum
2006 – 2007	Department of Chemistry, Ruhr Universität Bochum, Germany
2006 (Nov., Dec.)	Max Planck Institute for Physics of Complex Systems, Dresden

Grants Awarded:

07.01.23 – 06.30.26	National Science Foundation CHE-2245240, $465,089, "Modeling energy dynamics and thermal transport in molecules."
07.15.19 – 06.30.24	National Science Foundation CHE-1854271, $433,251, "Energy transfer in complex molecules."
06.15.14 – 09.30.19	National Science Foundation CHE-1361776, $423,546, "Thermal transport and rectification in molecules and nanoporous materials."
09.01.09 – 08.31.14	National Science Foundation CHE-0910669, $267,312, "Energy transport in proteins."
12.01.09 – 11.30.12	Volkswagen Foundation, $270,000 "Probing solvation dynamics of antifreeze proteins," (with M. Havenith, PI; M. Gruebele, co-PI).
05.01.05 – 04.30.10	National Science Foundation CHE-0512145, $333,000, "Vibrational dynamics of glasses and large molecules."
04.15.05 – 03.31.09	National Science Foundation OISE-0437165, $35,000, "Dynamical foundation of protein function." (NSF-JSPS cooperative grant; with R. S. Berry and J. E. Straub).

06.01.04 - 03.31.08 Human Frontier Science Program, $1,050,000, "Direct observation and modeling of protein motions important for function and folding," (co-PI with M. Gruebele and M. Havenith).

09.15.01 – 08.31.05 National Science Foundation CHE-0112631, $331,830, "Heat transport and chemical reactions in proteins and clusters."

Invited Talks:
(*List includes invited talks at scientific conferences, invited university talks, public lectures.)*

169. Biomolecular Sciences Seminar, Boise State University, September 2025.

168. Telluride Workshop, Vibrational Dynamics, Telluride Science Research Center, Telluride, CO, June 2025.

167. Telluride Workshop, Complex Kinetics and Dynamics from Single Molecules to Cells, Telluride Science Research Center, Telluride, CO, June 2025.

166. Department of Chemistry Seminar, UNLV, January 2025.

165. Sugadaira Winter Workshop, The Role of Fluctuations and Dynamics in Bio and Soft Matter, Sugadaira, Japan, January 2025.

164. Molecular Quantum Technology 2024, Puerto Varas, Chile, December 2024.

163. Energy Landscapes 2024, Lovran, Croatia, August 2024.

162. Ned Sibert's Retirement Symposium, University of Wisconsin, Madison, June 2024.

161. Workshop, Complex Kinetics and Dynamics from Single Molecules to Cells, University of Burgundy, Dijon, France, June 2024.

160. ACS Spring 2024, Vibrational Dynamics: Spectroscopy and Imaging Symposium, New Orleans, LA, March 2024.

159. Telluride Workshop, The Role of Fluctuations and Dynamics in Biomolecular Function, Telluride Science Research Center, January 2024.

158. International Conference on Molecular Energy Transfer in Complex Systems (iCOMET2023), Jaipur, India, November 2023.

157. Physical Chemistry Seminar, Indian Institute of Science, Bangalore, India, Nov. 2023.

156. Plenary Speaker, Theory and Applications of Computational Chemistry (TACC2023), Sapporo, Japan, September 2023.

155. Telluride Science Workshop, Vibrational Dynamics, Telluride, CO, July 2023.

154. RESOLV Summer School Solvation Science 2023, Ruhr-Universität Bochum, Germany, May 2023.

153. ACS Spring 2023, Peter Wolynes 70th Birthday Symposium, Indianapolis, IN, March 2023.

152. APS March Meeting, Focus Session on Intrinsically Disordered Proteins and Non-equilibrium Processes, Las Vegas, NV, March 2023.

151. Telluride Science Workshop, Energy Landscapes, Telluride, Colorado, July 2022.

150. University of Hamburg Photon Science Colloquium, Hamburg, Germany, July 2022.

149. Telluride Science Workshop, The Complexity of Dynamics and Kinetics from Single Molecules to Cells, June 2022.

148. Telluride Science Workshop, Thermal Transport at the Nanoscale, June 2022.

147. Telluride Science Workshop, Vibrational Dynamics (online), July 2021.

146. Telluride Science Workshop, Water Structure, Dynamics and Thermodynamics in Biology, (online), June 2021.

145. Department of Physics Seminar, University of Hamburg, Germany (online), June 2021.

144. Department of Chemistry Colloquium, Arizona State University (online), April 2021.

143. Physical Chemistry Seminar, University of Maryland (online), March 2021.

142. Telluride Science Summer Lecture Series (online), Aug. 2020.

141. Physical Chemistry Seminar, Institute for Molecular Science, Okazaki, Japan, December 2019.

140. Physics Department Seminar, Nara Women's University, Nara, Japan, December 2019.

139. Biophysics Seminar, Kyoto University, Kyoto, Japan, November 2019.

138. Physical Chemistry Seminar, Osaka University, Osaka, Japan, Nov. 2019.

137. Physical Chemistry Seminar, Tokyo Institute of Technology, Tokyo, Japan, Oct. 2019.

136. Physical Chemistry Seminar, RIKEN, Wako, Japan, Oct. 2019.

135. Biophysics Seminar, Nagoya University, Nagoya, Japan, Oct. 2019.

134. Workshop on Chemical Dynamics, Hokkaido University, Sapporo, Japan, Sept. 2019.

133. Biophysical Society of Japan Annual Meeting, Miyazaki, Japan, Sept. 2019.

132. Plenary speaker, XXXIX. Dynamics Days Europe Conference, Rostock, Germany, September 2019.

131. Telluride Workshop, Vibrational Dynamics, Telluride Sci. Research Center, July 2019.

130. Telluride Workshop, Thermal Transport at the Nanoscale, TSRC, June 2019.

129. Telluride Workshop, The Role of Fluctuations and Dynamics in Biomolecular Function, Telluride Science Research Center, Jan. 2019.

128. Department of Mechanical Engineering, University of Nevada, Reno, Dec. 2018.

127. Department of Pharmaceutical Sciences Seminar, University of California, Irvine, October 2018.

126. Physical Chemistry Seminar, University of California, Riverside, October 2018.

125. Department of Physics Seminar, Virginia Tech, Blacksburg, VA, October 2018.

124. Symposium on Theoretical Biochemistry, Euro Chemistry, Rome, Italy, June 2018.

123. Telluride Workshop, New Challenges for Theory in Chemical Dynamics, TSRC, January 2018.

122. Telluride Workshop, Vibrational Dynamics, Telluride Sci. Research Center, August 2017.

121. Telluride Workshop, Optimizing Thermodynamic Systems, TSRC, July 2017.

120. Telluride Workshop, Complexity of Dynamics and Kinetics from Single Molecules to Cells, TSRC, June 2017.

119. Center for Advanced Studies, University of Nevada – Reno, May 2017.

118. Department of Physics Seminar, Nagoya University, Nagoya, Japan, October 2016.

117. Telluride Workshop, Molecular Recognition and the Chemical Senses, TSRC, July 2016.

116. QSCP-XXI Symposium, New Frontiers of Chemical Dynamics, Vancouver, BC, July 2016.

115. Telluride Workshop, Thermal Transport at the Nanoscale, TSRC, June 2016.

114. Pacifichem Symposium on Quantum Coherence in Energy Transfer, Hawaii, Dec. 2015.

113. Telluride Workshop on Geometry of Chemical Reaction Dynamics in Gas and Condensed Phases, Telluride Sci. Research Center, August 2015.

112. Telluride Workshop on Vibrational Dynamics, Telluride Sci. Research Center, July 2015.

111. FRIAS Research Seminar, Research Focus Quantum Transport, Freiburg Institute for Advanced Studies, Freiburg, Germany, June 2015.

110. Telluride Workshop, R. Stephen Berry Tribute, Telluride Sci. Research Center, June 2015.

109. Biomolecular Dynamics Seminar, Freiburg University, Freiburg, Germany, June 2015.

108. Chemistry & Biochemistry Seminar, University of Notre Dame, South Bend, IN, Oct. 2014.

107. Telluride Workshop on Spectroscopy and Dynamics of Floppy Molecular Systems, Telluride Science Research Center, Telluride, CO, July 2014.

106. Natural Sciences Colloquium, Freiburg Institute for Advanced Studies, Freiburg, Germany, July 2014.

105. Physics Colloquium, University of Frankfurt, Frankfurt, Germany, June 2014.

104. Physics Colloquium, University of Freiburg, Freiburg, Germany, May 2014.

103. Les Houches – TSRC Protein Dynamics Workshop, Les Houches, France, May 2014.

102. Biophysics Seminar, University of California, Davis, Davis, CA, April 2014.

101. CECAM Workshop, Heat Transfer on Small Scales, Zaragoza, Spain, October 2013.

100. Chinese Academy of Sciences International Symposium on Physical Principles of Biomolecules, in honor of P. G. Wolynes and J. N. Onuchic, Beijing, PRC, August 2013.

99. Telluride Town Talk (Public lecture): “Smell: What triggers it?” Telluride, CO, July 2013.

98. Telluride Workshop on Vibrational Dynamics, Telluride Sci. Research Center, July 2013.

97. Telluride Workshop on Thermal Transport at the Nanoscale, TSRC, June 2013.

96. American Chemical Society National Meeting, New Orleans, LA, April 2013.

95. Physical Chemistry Seminar, University of Pennsylvania, Philadelphia, PA, January 2013.

94. Frontiers of THz Science, Stanford U. (SLAC), Palo Alto, CA, September 2012.

93. American Chemical Society National Meeting, Philadelphia, PA, August 2012.

92. Telluride Workshop on Interfacial Molecular Structure and Dynamics, TSRC, July 2012.

91. Theoretical Chemistry Seminar, MIT, March 2012.

90. Chemistry Faculty Research Seminar, Boston University, Feb. 2012.

89. Greater Boston Area Theoretical Chemistry Lecture Series, MIT, Jan. 2012.

88. 7th US-Japan Joint Seminar on Nanoscale Transport Phenomena, Shima, Japan, December 2011.

87. Biological Physics Seminar, Arizona State University, October 2011.

86. Theoretical Chemistry Seminar, Purdue University, Sept. 2011.

85. Physical Chemistry Seminar, Purdue University, Sept. 2011.

84. Telluride Workshop on Quantum Transport, Telluride Sci. Res. Center, Aug. 2011.

83. Telluride Workshop on Energy Landscapes, Telluride Sci. Res. Center, Aug. 2011.

82. Telluride Workshop on Vibrational Dynamics, Telluride Sci. Res. Center, July 2011.

81. Biomolecular Dynamics Seminar, Freiburg University, Freiburg, Germany, July 2011.

80. NSF Workshop on THz/IR Spectroscopy, Arlington, VA, April 2011.

79. Pacifichem Symposium on Spectroscopic Probes of Intermolecular Interactions, Honolulu, Hawaii, Dec. 2010.

78. Gordon Conference on Vibrational Spectroscopy, Maine, August 2010.

77. Physical Chemistry Seminar, Ruhr-Universität Bochum, Germany, July 2010.

76. Telluride Workshop on Thermal Transport at the Nanoscale, TSRC, June 2010.

75. Plenary Speaker, XXII Sitges Conference on Stat. Mechanics, Sitges, Spain, June 2010.

74. Department of Physics Seminar, Universite Libre de Bruxelles, Belgium, June 2010.

73. Leopoldina Conference on Water and Proteins, Ruhr-Universität Bochum, May 2010.

72. Chemistry Department Seminar, Tulane University, January 2010.

71. Telluride Workshop on Frontiers of Chemical Dynamics, TSRC, January 2010.

70. Telluride Workshop on Quantum Transport, TSRC, July 2009.

69. Telluride Workshop on Vibrational Dynamics, Telluride Sci. Research Center, July 2009.

68. Quantum Efficiency Seminar, Dept. of Physics, Freiburg University, Germany, June 2009.

67. Workshop on Proteins and Water, Arizona State University, Tempe, AZ, May 2009.

66. Biophysics Seminar, University of California, Davis, May 2009.

65. NSF-JSPS Workshop on Protein Dynamics, Sapporo, Japan, February 2009.

64. Advances in Chemical Dynamics Workshop, Santa Fe, NM, August 2008.

63. 6th Congress of International Society for Theor. Chem. Phys., U. British Columbia, July 2008.

62. Department of Physics, Nagoya University, Nagoya, Japan, February 2008.

61. Department of Chemistry Colloquium, Cornell University, Ithaca, NY, February 2008.

60. Telluride Workshop on Theory of Chemical Dynamics, Telluride Sci. Res. Center, January 2008.

59. Workshop on Computational Biophysics, Nagoya University, Nagoya, Japan, Nov. 2007.

58. Telluride Workshop on Vibrational Dynamics, Telluride Science Research Center, August 2007.

57. Physical Chemistry Institute, Universität Heidelberg, Heidelberg, Germany, May 2007.

56. Bunsen Discussion Meeting, "Exploring THz Spectroscopy", Bad Honnef, Germany, April 2007.

55. Department of Chemistry Colloquium, Ruhr-Universität Bochum, Germany, April 2007.

54. American Chemical Society National Meeting, Chicago, March 2007.

53. Conference on "Spectroscopy and Dynamics of Molecules and Clusters" (SDMC 07), Uttarkhand, India, Feb. 2007.

52. Fritz Haber Institute, Hebrew University, Jerusalem, Israel, Feb. 2007.

51. Physical Chemistry Institute, Universität Frankfurt, Frankfurt, Germany, Jan. 2007.

50. Physical Chemistry Institute, Universität Bielefeld, Bielefeld, Germany, Jan. 2007.

49. Max Planck Inst. for Physics of Complex Systems Colloquium, Dresden, Germany, December 2006.

48. Max Planck Institute for Biochemistry, Göttingen, Germany, Dec. 2006.

47. Conference on "Multimode Dynamics", Universität Heidelberg, Germany, Nov. 2006.

46. Physical Chemistry Institute, Universität Zürich, Zürich, Switzerland, Nov. 2006.

45. Southwest Regional Meeting of the American Chemical Society, Houston, October 2006.

44. American Chemical Society National Meeting, San Francisco, September 2006.

43. Gordon Conference on Vibrational Spectroscopy (Discussion Leader), Maine, July 2006.

42. Department of Chemistry, University of Wisconsin, Madison, January 2006.

41. Biophysical Society of Japan National Meeting, Sapporo, Japan, Nov. 2005.

40. Telluride Workshop on Energy Landscapes, Telluride, CO, August 2005.

39. Telluride Workshop on Vibrational Dynamics in Condensed and Gas Phases, Aug. 2005.

38. Department of Physics, Bilkent University, Ankara, Turkey, June 2005.

37. Theoretical Biophysics Seminar, University of California, San Diego, June 2005.

36. American Physical Society National Meeting, Los Angeles, March 2005.

35. Department of Chemistry, University of Colorado, Boulder, January 2005.

34. Workshop on "Energy Localization: From Small Polyatomics to Large Biomolecules," CECAM, Lyon, France, September, 2004.

33. Physical Chemistry Institute, Ruhr Universität Bochum, June 2004.

32. Department of Chemistry, University of Oregon, May 2004.

31. Department of Chemistry, The Ohio State University, April 2004.

30. Department of Chemistry, University of Cincinnati, April 2004.

29. Department of Chemistry, University of Illinois at Urbana-Champaign, April 2004.

28. Department of Chemistry, University of California, Irvine, March 2004.

27. Conference on "Chemical reaction dynamics in complex systems," Yukawa Institute, Kyoto, Japan, Oct. 2003.

26. Conference on "Geometrical structures in phase space," Kobe, Japan, Oct. 2003.

25. Department of Chemistry, University of California, Davis, October 2003.

24. Telluride Workshop on Vibrational Dynamics in Gas and Condensed Phases, August 2003.

23. Telluride Workshop on Energy Landscapes, Telluride, CO, July 2003.

22. Conference on "Quantum transport," Bad Honnef, Germany, March 2003.

21. Workshop on "Teaching Across the Physical Sciences," U. of Chicago, June 2002.

20. Department of Physics, University of Nevada, Reno, February 2002.

19. Department of Physics, University of Georgia, Athens, GA, February 2002.

18. Department of Chemistry, University of Maryland, Baltimore Co., December 2001.

17. Department of Mathematics, University of Nevada, Reno, November 2001.

16. Department of Chemistry, Bilkent University, Ankara, Turkey, January 2001.

15. Department of Chemistry, University of Michigan, Ann Arbor, MI, February 2000.

14. Faculty of Science, Bilkent University, Ankara, Turkey, December 1999.

13. Physical Chemistry Institute, Universität Heidelberg, Heidelberg, Germany, November 1999.

12. Department of Chemistry, Cambridge University, Cambridge, England, October 1999.

11. American Chemical Society National Meeting, Anaheim, CA, March 1999.

10. Sanibel Symposium, University of Florida, Gainesville, FL, February 1999.

9. Department of Physics, University of Athens, Athens, Greece, November 1998.

8. Telluride Workshop on Quantum Control, Telluride, CO, July 1998.

7. Condensed Matter Seminar, U. of Illinois at Urbana-Champaign, April 1998.

6. Telluride Workshop on Vibrational Dynamics, Telluride, CO, July 1997.

5. Department of Chemistry, MIT, Cambridge, MA, January 1997.

4. Telluride Workshop on Vibrational Dynamics, Telluride CO, July 1996.

3. Department of Chemistry, University of Wisconsin-Madison, April 1996.

2. Department of Chemistry, University of Cincinnati, October 1995.

1. Telluride Workshop on Vibrational Dynamics, Telluride, CO, July 1995.

Organization of Professional Meetings:

14. Pacifichem Symposium, "Biomolecules at interfaces defining the cellular environment: From conformational dynamics to informatics approaches," Pacifichem 2025, Honolulu, Hawaii (with Masataka Nagaoka, Nagoya U.; John Straub, BU; Changbong Hyeon, Korea Institute for Advanced Study (KIAS)).

13. West Coast Theoretical Chemistry Meeting 2025, University of Nevada, Reno, May 10, 2025 (with S. Varganov, S. Odoh, D. Cantu, M. Fizer, T. Tscherbul)

12. ACS National Meeting, "Peter G. Wolynes 70th Birthday Symposium," Indianapolis, IN, March 26 – 30, 2023 (with J. Wang, Stony Brook; B. Zhang, MIT; Garegin Papoian, U. Maryland; Vassiliy Lubchenko, U. Houston).

11. Pacifichem Symposium, "Biomolecules at interfaces defining the cellular environment: From conformational dynamics to informatics approaches," Pacifichem 2020 (postponed to 2021), Honolulu, Hawaii (with Masataka Nagaoka, Nagoya U.; John Straub, BU; Changbong Hyeon, Korea Institute for Advanced Study (KIAS)).

10. Annual Meeting of the Biophysical Society of Japan Symposium, "Structure, Dynamics and Energy Flow that Govern Heme Protein Functions: Theory and Experiments," Miyazaki, Japan, Sept. 24 - 16, 2019 (with Takahisa Yamato, Nagoya University).

9. CECAM Workshop, "Network analysis to elucidate natural system dynamics, diversity and performance," Lyon, France, May 2 – 4, 2019 (with Claire Lesieur, Lyon; Luisa Di Paula, Rome; Alessandro Giuliani, Rome; Elena Papaleo, Copenhagen).

8. Pacifichem Symposium, "Conformational dynamics of biomolecules and the biomolecule-solvent interface," Pacifichem 2015, Honolulu, Hawaii, Dec. 15 – 20, 2015 (with Masataka Nagaoka, Nagoya U.; John Straub, BU; YiQin Gao, Peking U.).

7. Annual Meeting of the Far West Section of the American Physical Society, Reno, NV, October 24 – 25, 2014 (member of local organizing committee).

6. TSRC Workshop, "Thermal transport at the nanoscale," Telluride Science Research Center, Telluride, CO, June 25-29, 2013 (with Alan McGaughey, Carnegie-Mellon University).

5. TSRC Workshop, "Thermal transport at the nanoscale," Telluride Science Research Center, Telluride, CO, June 21-15, 2010 (Co-creator of workshop, with Alan McGaughey, Carnegie-Mellon University).

4. Bunsen Discussion Meeting, "Exploring THz Spectroscopy", Phyzikzentrum, Bad Honnef, Germany, Apr. 2-4, 2007 (with Martina Havenith, Bochum; Charles Schmuttenmaer, Yale).

3. ACS Theoretical/Computational Chemistry Symposium, American Chemical Society Northwest Regional Meeting, June 26-27, 2006 (with Hyung-June Woo, U. Nevada, Reno).

2. TSRC Workshop, "Vibrational dynamics in condensed and gas phases," Telluride Science Research Center, Telluride, CO, August 8-12, 2005 (with Peter Hamm, U. of Zürich).

1. APS Focus Session, "Energy landscapes of biomolecules," American Physical Society National Meeting, Los Angeles, CA, March 21-25, 2005 (with Martin Gruebele, U. Illinois).

High School, Undergraduate and Graduate Advisor and Postgraduate-Scholar Sponsor:

High School Students: Matt Enright, Mia Swain, Jessica Wei.

Undergraduates: Reya Kempley, David Ponte, Chantal Reyna, Patrick Tomco, Ben Borgo, Amber Jain, Taylor Kaplan, Marcus Sacchetti, Marie Jones, James Ludwig, Yuxin Jiang.

Graduate Students: Johnson Agbo, Yao Xu, Hari Pandey, Korey Reid, David Kirkland, Humanath Poudel, Pathick Halder.

Postdoctoral Associates: Xin Yu, Gia Maisuradze, J. Park, R. Gnanasekaran, Pritom Bose.

Faculty and Students Hosted:

Fulbright Research Fellow: Prof. Luisa Di Paola, Università Campus Biomedico Rome, Italy, 2022.
DAAD short-term doctoral fellow: Matthias Heyden, Ruhr-Universität Bochum, Germany, 2006.

Courses Taught:

CHEM 121, General Chemistry 1 (Spring 2005, Spring 2010, Spring 2021, Spring 2025)
CHEM 202, Freshman Chemistry for Scientists and Engineers (Spring 2001)
CHEM 422, Physical Chemistry II (Spring 2013, 2014, 2015, 2017, 2019)
CHEM 425*, Biophysical Chemistry (Fall 2001, 2002, 2003, 2004, 2007, ‘10, ‘11, ‘12, ’17, ’25)
CHEM 655, (Boston University) Statistical Mechanics (Spring 2012)
CHEM 751, Non-Equilibrium Statistical Mechanics (Spring 2009, Fall 2021)
CHEM 754, Molecular Spectroscopy (Spring 2002, Fall 2005, 2009, 2013, 2015, 2023)
CHEM 755, Statistical Thermodynamics (Spring ‘04, ‘06, ‘08, ‘16, ‘18, ‘20, ‘22, ‘24)
CHEM 757, Quantum Chemistry (Fall ‘00, ‘02, ‘08, ‘10, ‘14, ‘16, ‘18, ‘20, ‘22, ‘24)

* DML created this 1-semester physical chemistry course for students in the biochemical/biological sciences as an alternative to Physical Chemistry I.

Service and Professional Activities:

University of Nevada, Reno

Director, Center for Advanced Studies (2018 – 2024)
Director, Chemical Physics Program (2009 – 2017)
Center for Advanced Studies Executive Committee (2016 – present)
UNR Outstanding Researcher Award Committee (2015 – 2019, 2022, 2023)
Nevada Regents’ Distinguished Researcher Award (2016 – 17, 2023 – 24)
Mousel-Feltner Award Committee (2005, 2006, 2008, 2010)
Shin Award Committee (2012, 2025)
College of Science Personnel Committee (2009 – 12, 2024 – 27)
College of Science Graduate Council Representative (2024 – 25)
College of Science Research Computing Committee (2013 – 2015)
Physics Department Faculty Search Committee, Member (2014 – 15, 2016 - 17)
College of Science Research Computing Administrator Search Comm., Member (2014 – 15)
Chemistry Department Graduate Recruitment Committee (2000 – 2004)
Chemistry Department Computing Coordinator (2000 – 2004)
Chair, Chem. Department Computing and Instrumentation Committee (2004 – 2005)
Chemistry Dept. Faculty Search Committee (2003 – 2004, 2012 – 2013, 2022 - 2023)
Chair, Chemistry Department Publicity and Alumni Relations Committee (2005 - 2012)
Physical Chemistry Seminar Coordinator (2004 – 2006, 2008 - 2010)
Physical Chemistry Division Liaison (2007 – 2015)

Chair, Chemistry Department Theory Search Committee (2010 - 2011)

American Chemical Society

Physical Chemistry Division Executive Committee Member-at-Large (2017 – 2019)

American Physical Society

Division of Chemical Physics Nominating Committee (2020, 2021 (as Chair))
Division of Chemical Physics Secretary/Treasurer (2010 – 2013)

The Journal of Chemical Physics

Editorial Advisory Board (2016 – 2018)

Scientific Reports - Nature

Editorial Board (2017 – present)

Entropy

Editorial Board (2022 – present)

The Journal of Physical Chemistry A/B/C

Editorial Advisory Board (2019 – 2021)

Telluride Science Research Center

Member of the Board (2005-2007); Nominating Committee, Chair (2011)

Pinhead Institute, Telluride, CO (Smithsonian Affiliate)

Pinhead Punk Science Presenter (2009)

Davidson Academy of Nevada

Science Olympiad Coach (2012 – 2020)

Intel International Science and Engineering Fair

Grand Award Judge (2014, 2015)

American Chemical Society Sierra Nevada Section

Secretary/Treasurer (2002), Chair-Elect (2003), Chair (2004)

Reviewer

(Excluding multiple tenure and promotion reviews): *J. Phys. Chem. A, B, C & Lett.; J. Chem. Phys.; Phys. Chem. Chem. Phys.; Chem. Phys. Lett.; Chem. Phys.; ChemPhysChem; J. Comp. Theor. Chem.; Physical Review Letters, Phys. Rev. B & E; New. J. Phys.; J. Phys.: Cond. Mat.; J. Appl. Phys.; Biophys. J.; Biochemistry; Biopolymers; Theochem.; Proteins; J. Royal Soc. Interface; JACS; Angew. Chem.; Small; Nature Nanotech.; Sci. Rep.; Nature Comm.; PNAS; Science; Nature;* Taylor & Francis; Springer; *Physics Today*; National Science Foundation; American Chem. Soc.; Dept. of Energy; Human Frontier Science Program; M. J. Murdoch Trust; Natural Sci. and Eng. Res. Council (Canada); European Research Council; Agence Nationale de la Recherche (France); Israel Science Foundation; National Science Centre, Poland; Austrian Science Fund; FONDECYT-Chile; Freiburg Institute for Advanced Studies.

Named among the Journal of Chemical Physics Top 20 Reviewers for 2012

National Science Foundation panelist

CRIF; Chem. Theory, Models & Comp. Methods; Chem. of Life Processes

Membership: AAAS (Fellow), ACS, American Physical Society (Fellow)

List of Publications

Google Scholar: https://scholar.google.com/citations?user=hbcekPYAAAAJ&hl=en

Books edited:

Advancing Theory for Kinetics and Dynamics of Complex Many Dimensional Systems: Clusters and Proteins, T. Komatsuzaki, R. S. Berry, D. M. Leitner, eds., *Adv. Chem. Phys.* **145** (Wiley, Hoboken, 2011).

Proteins: Energy, Heat and Signal Flow, D. M. Leitner and J. E. Straub, eds. (Taylor and Francis Press, Boca Raton, 2009).

Articles:

151. "Perspective: The microcanonical Lindemann mechanism for unimolecular reactions," D. M. Leitner, *J. Chem. Phys.* (accepted).

150. "Modulating vibrational energy redistribution in highly conjugated systems," M. Hassani, P. H. Shaon, C. J. Mallon, T. Shi, J. N. Monzy, E. E. Fenlon, D. M. Leitner, M. J. Tucker, *J. Chem. Phys.* **162**, 154201 (2025) (David Jonas Festschrift).

149. "Internal vibrational energy redistribution precedes energy dissipation into the solvent upon photoexcitation of heme proteins," A. Buchmann, L. Caminiti, L. L. Stiewe, S. Jung, D. M. Leitner, M. Havenith, *Phys. Chem. Chem. Phys.* **27**, 9470 – 9477 (2025).

148. "Tuning vibrational lifetimes by chemical substitution and impact on plasmon-assisted catalysis," P. H. Shaon, H. Poudel, D. M. Leitner, *J. Phys. Chem. A* **129**, 2006 – 2015 (2025).

147. "Temperature dependence of thermal conductivity of proteins: Contributions of thermal expansion and Grüneisen parameter," D.M. Leitner, *ChemPhysChem*, **26**, e202401017 (2025) (Part of special issue, "Physical Chemistry in North America").

146. "A strategy for modeling nonstatistical reactivity effects: Combining chemical activation estimates with a vibrational relaxation model," T. Rožić, M. S. Teynor, N. Došlić, D.M. Leitner, G.C. Solomon, *J. Chem. Theory Comput.* **20**, 9048 – 9059 (2024).

145. "Vibrational energy landscapes and energy flow in GPCRs," by H. Poudel, D. J. Wales and D. M. Leitner *J. Phys. Chem. B* **128,** 7568 – 7576 (2024) (Richard J. Saykally Festschrift).

144. "Vibrational energy flow in molecules attached to plasmonic nanoparticles" by H. Poudel, P. H. Shaon and D. M. Leitner *J. Phys. Chem. C* **128**, 8628 – 8636 (2024).

143. "What measurements of energy transfer across non-covalent contacts in proteins reveal about the energy landscape," H. Poudel, D. M. Leitner, *J. Innovative Materials in Extreme Conditions* **5**, 45 – 56 (2024) (J. Christian Schön Festschrift).

142. "Dynamics of hydrogen bonds between water and intrinsically disordered and structured regions of proteins," K. M. Reid, H. Poudel, D. M. Leitner, *J. Phys. Chem. B.* **127**, 7839 - 7847 (2023).

141. “Locating dynamic contributions to allostery via determining rates of vibrational energy transfer,” H. Poudel, D. M. Leitner, *J. Chem. Phys.* **158**, 015101 (2023) (Part of special topic issue, “New Views of Allostery”).

140. “Energy transport in class B GPCRs: Role of protein-water dynamics and activation,” H. Poudel, D. M. Leitner, *J. Phys. Chem. B* **126**, 8362 – 8373 (2022).

139. “Enhanced mobility during Diels-Alder reaction: Results of molecular simulations,” K. M. Reid, D. M. Leitner*, J. Phys. Chem. Lett*. **13**, 3763-3769 (2022).

138. “A statistical journey through the topological determinants of the b2 adrenergic receptor dynamics,” L. Di Paola, H. Poudel, M. Parise, A. Giuliani, D. M. Leitner, *Entropy* 24, art. no. 998 (2022).

137. “Biophysical insight into the SARS-CoV2 Spike-ACE2 interaction and its modulation by hepcidin through a multifaceted computational approach,” H. Hadi-Alijanvand, L. Di Paola, G. Hu, D. M. Leitner, G. M. Verkhivker, P. Sun, H. Poudel, A. Giuliani, *ACS Omega*, **7**, 17024 – 17042 (2022).

136. “The origin and impact of bound water around intrinsically disordered proteins,” K. M. Reid, A. K. Singh, C. R. Bikash, J. Wei, Y. Tal-Gan, N. Q. Vinh, D. M. Leitner, *Biophysical Journal* **121**, 540 – 551 (2022).

135. “Richard Stephen Berry (1931 – 2020)”, Srihari Keshavamurthy, Tamiki Komatsuzaki, David Leitner, *Resonance* **27** (1), 11 – 17 (2022).

134. “Electric fields influence intramolecular energy relaxation and line widths”, A. Maitra, S. Sarkar, D. M. Leitner, J. M. Dawlaty*, J. Phys. Chem. Lett*. **12**, 7818-7825 (2021).

133. “Activation-induced reorganization of energy transport networks in the β_2 adrenergic receptor,” H. Poudel, D. M. Leitner, *J. Phys. Chem. B* **125**, 6522 – 6531(2021) (Part of special issue, “125 Years of *The Journal of Physical Chemistry*”).

132. “Change in vibrational entropy with change in protein volume estimated with mode Grüneisen parameters,” K. M. Reid, X. Yu, D. M. Leitner, *J. Chem. Phys*. 154, art. no. 055102 (2021).

131. “Network models of biological adaptation at the molecular scale: Comment on ‘Dynamic and thermodynamic models of adaptation’ by A.N. Gorban, *et al*.,” L. Di Paola, D. M. Leitner, *Physics of Life Rev*iews **38**, 124 – 126 (2021).

130. “Locating and navigating energy transport networks in proteins,” K. M. Reid, D. M. Leitner, in *Allostery, Methods in Molecular Biology*, L. Di Paola, A. Giuliani, eds.; Springer, 2021; vol. 2253, Ch. 4, pp. 37 - 59.

129. “Water-mediated biomolecular dynamics and allostery,” D. M. Leitner, C. Hyeon, K. M. Reid, *J. Chem. Phys*. 152, art. no. 240901 (2020) (Perspective article; Featured article).

128. “Energy transfer across nonpolar and polar contacts in proteins: Role of contact fluctuations,” H. Poudel, K. M. Reid, T. Yamato, D. M. Leitner, *J. Phys. Chem. B* 124, 9852 – 9861 (2020) (Yoshitaka Tanimura Festschrift).

127. “Variation of energy transfer rates across protein-water contacts with equilibrium structural fluctuations of a homodimeric hemoglobin,” K. M. Reid, T. Yamato, D. M. Leitner, *J. Phys. Chem. B* **124**, 1148 – 1159 (2020) (ACS Editors’ Choice).

126. “Recent developments in the computational study of protein structural and vibrational energy dynamics,” D. M. Leitner, T. Yamato, *Biophys. Rev*. **12**, 317 – 322 (2020).

125. “Structure, dynamics and energy flow that govern heme protein functions: theory and experiments,” T. Yamato, D. M. Leitner, *Biophys. Rev*. (2020). DOI:10.1007/s12551-020-00625-4.

124. “Tuning molecular vibrational energy flow within an aromatic scaffold via anharmonic coupling,” A. J. Schmitz, H. D. Pandey, F. Chalyavi, T. Shi, E. E. Fenlon, S. H. Brewer, D. M. Leitner, M. J. Tucker, *J. Phys. Chem. A* **123**, 10571-10581 (2019).

123. “Energy transport across interfaces in biomolecular systems,” D. M. Leitner, H. D. Pandey, K. M. Reid, *J. Phys. Chem. B* **123**, 9507 – 9524 (2019) (Feature Article; ACS Editors’ Choice).

122. “Elastic and inelastic contributions to thermal transport between chemical groups and thermal rectification in molecules,” K. M. Reid, H. D. Pandey and D. M. Leitner, *J. Phys. Chem. C* **123**, 6256 - 6264 (2019) (Abraham Nitzan Festschrift).

121. “Illuminating Fermi resonances that trigger reaction in a complex molecule,” D. M. Leitner, *Chem* **5**, 256 - 257 (2019).

120. “Molecules and the Eigenstate Thermalization Hypothesis,” D. M. Leitner, *Entropy* **20**, art. 673, pp. 1 - 17 (2018) (Feature Paper, special issue, “Quantum Ergodicity”).

119. “Scaling of rates of vibrational energy transfer in proteins with equilibrium dynamics and entropy,” K. M. Reid, T. Yamato, D. M. Leitner, *J. Phys. Chem. B* **122**, 9331 – 9339 (2018) (Special issue, “Deciphering Molecular Complexity in Dynamics and Kinetics from the Single Molecule to the Single Cell Level”). https://pubs.acs.org/doi/10.1021/acs.jpcb.8b07552

118. “Vibrational states and nitrile lifetimes of cyanophenylalanine isotopomers in solution,” H. D. Pandey and D. M. Leitner, *J. Phys. Chem. A* **122**, 6856 – 6863 (2018) (William Reinhardt Festschrift).

117. “Hydrophobic collapse of ubiquitin generates rapid protein-water motions,” H. Wirtz, S. Schäfer, C. Hoberg, K. M. Reid, D. M. Leitner, M. Havenith, *Biochemistry* **57**, 3650 - 3657 (2018).

116. “Small saccharides as a blanket around proteins: A computational study,” H. D. Pandey and D. M. Leitner, *J. Phys. Chem. B* **122**, 7277 - 7285 (2018).

115. “Mapping energy transport networks in proteins,” D. M. Leitner and T. Yamato, in *Reviews in Computational Chemistry*, A. L. Parrill, K. B. Lipkowitz, eds.; Wiley, 2018; vol. 31, Ch. 2, pp. 63 – 113.

114. “Energy relaxation and thermal transport in molecules,” by D. M. Leitner, in *Handbook of Materials Modeling*, W. Andreoni and S. Yip, eds. (Springer: Cham, 2018).

113. “Thermodynamics of hydration water around an antifreeze protein: A molecular simulation study,” H. D. Pandey and D. M. Leitner, *J. Phys. Chem. B* **121**, 9498 - 9507 (2017).

112. “Influence of thermalization on thermal conduction through molecular junctions: Computational study of PEG oligomers,” H. D. Pandey and D. M. Leitner, *J. Chem. Phys.* **147**, art. 084701, pp. 1 - 11 (2017).

111. “Vibrational energy transport in molecules and the statistical properties of vibrational modes,” H. D. Pandey and D. M. Leitner, *Chem. Phys.* **482**, 81 – 85 (2017) (Lorenz Cederbaum Festschrift).

110. “Thermalization and thermal transport in molecules,” H. D. Pandey and D. M. Leitner, *J. Phys. Chem. Lett.* **7**, 5062 – 5067 (2016).

109. “Water–mediated energy dynamics in a homodimeric hemoglobin,” D. M. Leitner, *J. Phys. Chem. B* **120**, 4019 – 4027 (2016).

108. “Hydrophobic collapse induces changes in the collective protein and hydration low frequency modes,” T. Q. Luong, Y. Xu, E. Bründermann, D. M. Leitner, M. Havenith, *Chem. Phys. Lett*. **651**, 1 – 7 (2016) (Frontiers Article).

107. “Scaling rules for vibrational energy transport in globular proteins,” S. Buchenberg, D. M. Leitner, G. Stock, *J. Phys. Chem. Lett*. **7**, 25 – 30 (2016).

106. “Protein-water dynamics in antifreeze protein III activity,” Y. Xu, A. Bäumer, K. Meister, C. Bischak, A. L. DeVries, D. M. Leitner, M. Havenith, *Chem. Phys. Lett*. **647**, 1 – 6 (2016) (Frontiers Article).

105. “Quantum ergodicity and energy flow in molecules,” D. M. Leitner, *Advances in Physics* **64**, 445 – 517 (2015).

104. “Asymmetric energy flow in liquid alkylbenzenes: A computational study,” D. M. Leitner and H. D. Pandey, *J. Chem. Phys.* **143,** art. 144301, pp. 1 - 9 (2015).

103. “Quantum bottlenecks and unidirectional energy flow in molecules,” D. M. Leitner, H. D. Pandey, *Ann. der Phys.* **527**, 601 – 609 (2015) (Special Issue: Complex Quantum Systems).

102. “Vibrational energy flow in the villin headpiece subdomain: Master equation simulations,” D. M. Leitner, S. Buchenberg, P. Brettel, G. Stock, *J. Chem. Phys.* **142**, art. 075101, pp. 1 – 9 (2015).

101. “The size-dependent accuracy of nanoscale thermometers,” R. Alicki, D. M. Leitner, *J. Phys. Chem. B* **119**, 9000 – 9005 (2015).

100. “Thermal conductance at the interface between molecules,” D. M. Leitner, *Adv. Chem. Phys*. **157**, 159 – 164 (2015).

99. “The role of sulfates on antifreeze protein activity,” K. Meister, J. G. Duman, Y. Xu, A. L. DeVries, D. M. Leitner, M. Havenith, *J. Phys. Chem. B* **118**, 7920 – 2924 (2014).

98. “Vibrational energy flow across heme-cytochrome c and cytochrome c-water interfaces,” J. K. Agbo, Y. Xu, P. Zhang, J. E. Straub, D. M. Leitner, *Theo. Chem. Acc.* **133**, art. 1504, pp. 1-7 (2014). (Greg Ezra Festschrift)

97. “Communication maps: Exploring energy transport through proteins and water,” J. Agbo, R. Gnanasekaran, D. M. Leitner, *Israel J. Chem.* **54**, 1065 – 1073 (2014). (Special Issue: Computational Molecular Biophysics: 40 Years of Achievements, in honor of the 2013 Nobel Prize in Chemistry awarded to Martin Karplus, Michael Levitt and Arieh Warshel.)

96. “Communication maps of vibrational energy transport through photoactive yellow protein,” Y. Xu, D. M. Leitner, *J. Phys. Chem. A* **118**, 7280 – 7287 (2014). (Ken Jordan Festschrift)

95. “Vibrational energy flow through green fluorescent protein-water interface: Communication maps and thermal boundary conductance,” Y. Xu, D. M. Leitner, *J. Phys. Chem. B* **118**, 7818 – 7826 (2014). (Jim Skinner Festschrift)

94. “Thermal boundary conductance and thermal rectification in molecules,” D. M. Leitner, *J. Phys. Chem. B* **117**, 12820 – 828 (2013). (Peter Wolynes Festschrift)

93. “Long-range protein–water dynamics in hyperactive insect antifreeze proteins,” K. Meister, S. Ebbinghaus, Y. Xu, J. G. Duman, A. DeVries, M. Gruebele, D. M. Leitner, M. Havenith, *Proc. Natl. Acad. Sci. (USA)* **110**, 1617 – 22 (2013).

92. “The dielectric response to photoexcitation of GFP: A molecular dynamics study,” Y. Xu, R. Gnanasekaran, D. M. Leitner, *Chem. Phys. Lett*. **564**, 78 – 82 (2013).

91. “Mode damping rates in a protein chromophore,” D. M. Leitner, *Chem. Phys. Lett*, **530**, 102 – 106 (2012).

90. “Analysis of water and hydrogen bond dynamics at the surface of an antifreeze protein,” Y. Xu, R. Gnanasekaran and D. M. Leitner, *J. At. Mol. Opt. Phys.* **2012**, art. 125071, 1 – 6 (2012). (For special issue on Energy Landscapes, R. S. Berry, T. Komatsuzaki, D. J. Wales, eds.)

89. “THz technology and THz spectroscopy: Modeling and experiments to study solvation dynamics of biomolecules,” D. M. Leitner, M. Gruebele, M. Havenith, in *Methods in Physical Chemistry*, R. Schäfer, P. C. Schmidt, eds. (Wiley-VCH Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 2012), doi: 10.1002/9783527636839.ch22.

88. “Dielectric response and vibrational energy relaxation in photoactive yellow protein: A molecular dynamics simulation study,” R. Gnanasekaran and D. M. Leitner, *Chem. Phys. Lett.* **516**, 102 - 105 (2011).

87. “Communication maps computed for homodimeric hemoglobin: Computational study of water-mediated energy transport in proteins,” R. Gnanasekaran, J. K. Agbo and D. M. Leitner, *J. Chem. Phys.* **135**, art. No. 065103, pp 1 - 10 (2011) **[2011 JCP Editors’ Choice Article. One of 80 articles selected for JCP’s 80th anniversary collection.]**

86. “Dynamical tunneling from the edge of vibrational state space of large molecules,” D. M. Leitner, in *Dynamical Tunneling*, S. Keshavamurthy and P. Schlagheck, Eds. (Taylor and Francis Press, Boca Raton, 2011), pp. 211 - 224.

85. “Non-Brownian phase space dynamics of molecules, the nature of their vibrational states and non-RRKM kinetics,” D. M. Leitner, Y. Matsunaga, A. Shojiguchi, C.-B. Li, T. Komatsuzaki and M. Toda, *Adv. Chem. Phys*. **145**, 83 – 122 (2011).

84. “Dynamics of water clusters confined in proteins: A molecular dynamics simulation study of interfacial waters in a dimeric hemoglobin,” R. Gnanasekaran, Y. Xu and D. M. Leitner, *J. Phys. Chem. B* **114**, 16989 – 16996 (2010).

83. “Quantum localization, dephasing and vibrational energy flow in a *trans*-formanilide (TFA)-H_2O complex,” J. K. Agbo, A. Jain, and D. M. Leitner, *Chem. Phys*. **374**, 111 – 117 (2010). (Horst Köppel Festschrift)

82. “Quantum localization and protein-assisted vibrational energy flow in cofactors,” D. M. Leitner, *New J. Phys*. **12**, art. No. 085004, pp. 1 – 17 (2010).

81. “Rattling in the cage: Ions as probes of sub-picosecond water network dynamics,” D. A. Schmidt, Ö. Birer, S. Funkner, B. Born, R. Gnanasekaran, G. W. Schwaab, D. M. Leitner and M. Havenith, *J. Am. Chem. Soc*. **131**, 18512 – 18517 (2009).

80. “THz technology and THz spectroscopy: Modeling and experiments to study solvation dynamics,” D. M. Leitner, M. Gruebele and M. Havenith, Bunsen-Magazin **5**, 184 – 194 (2009) **(Cover Article).**

79. “Frequency resolved communication maps for proteins and other nanoscale materials,” D. M. Leitner, *J. Chem. Phys*. **130**, 195101-1-9 (2009).

78. “Heat transport in proteins,” D. M. Leitner, in: *Energy flow in proteins: Computational strategies to explore signaling, energy redistribution and heat flow*, D. M. Leitner and J. E. Straub, eds., (Taylor and Francis Press, Boca Raton, 2009), pp. 249 - 271.

77. “Solvation dynamics of biomolecules: modeling and terahertz experiments,” D. M. Leitner, M. Gruebele, M. Havenith, *HFSP Journal* (Perspective for special issue on protein folding dynamics) **2**, 314 - 323 (2008).

76. “Energy flow in proteins,” D. M. Leitner, *Ann. Rev. Phys. Chem*. **59**, 233 – 259 (2008).

75. “A quantum model of restricted vibrational energy flow on the way to the transition state in unimolecular reactions,” D. M. Leitner and M. Gruebele, *Mol. Phys*. **106,** 433 – 442 (2008) (**Cover Article** of Raphy Levine Festschrift).

74. “The long range influence of carbohydrates on the solvation dynamics of water – answers from THz spectroscopic measurements and molecular modelling simulations,” M. Heyden, U. Heugen, G. Niehues, E. Bründermann, D. M. Leitner, M. Havenith *J. Am. Chem. Soc*. **130**, 5773 - 5779 (2008).

73. “Protein sequence- and pH-dependent hydration probed by terahertz spectroscopy,” S. Ebbinghaus, S. J. Kim, M. Heyden, X. Yu, M. Gruebele, D. M. Leitner, M. Havenith, *J. Am. Chem. Soc*. **130**, 2374 – 2375 (2008).

72. “Quantum energy flow and the kinetics of water shuttling between hydrogen bonding sites on *trans*-formanilide,” J. K. Agbo, D. M. Leitner, E. M. Myshakin, and K. D. Jordan, *J. Chem. Phys.* **127**, art. 064315, pp. 1 – 10 (2007).

71. “An extended dynamical solvation shell around proteins,” S. Ebbinghaus, S.-J. Kim, M. Heyden, X. Yu, U. Heugen, M. Gruebele, D. M. Leitner, and M. Havenith, *Proc. Natl. Acad. Sci. USA* **104**, 20749 – 20752 (2007).

70. “Normal mode analysis and calculation of the cooling rates of the chromophore vibrations during isomerization of photoactive yellow protein,” G. G. Maisuradze, X. Yu and D. M. Leitner, *J. Biolog. Phys. Chem*. **7**, 25 – 29 (2007).

69. “Free energy landscape of a biomolecule in dihedral principal component space: Sampling convergence and correspondence between structures and minima,” G. G. Maisuradze and D. M. Leitner, *PROTEINS: Structure, Function and Bioinformatics* **67**, 569 – 578 (2007).

68. “Biomolecule large amplitude motion and solvation dynamics: Modeling and probes from THz to X-rays,” D. M. Leitner, M. Havenith and M. Gruebele, *Int. Rev. Phys. Chem.* **25**, 553 – 582 (2006).

67. “Thermal conductivity computed for vitreous silica and methyl-doped silica above the plateau,” X. Yu and D. M. Leitner, *Phys. Rev. B* **74**, art. 184305, pp. 1-11 (2006).

66. “Hydration dependence of the mass fractal dimension and anomalous diffusion of vibrational energy in proteins,” M. B. Enright, X. Yu and D. M. Leitner, *Phys. Rev. E* **73**, art. 051905, pp. 1-9 (2006).

65. “Quantum theory of enhanced unimolecular reaction rates below the ergodicity threshold,” D. M. Leitner and P. G. Wolynes, *Chem. Phys.* **329**, 163 – 167 (2006). (Lorenz Cederbaum Festschrift)

64. “Solute induced retardation of water dynamics: Hydration water probed directly by THz spectroscopy,” U. Heugen, G. Schwaab, E. Bründermann, M. Heyden, X. Yu, D. M. Leitner, and M. Havenith, *Proc. Nat. Acad. Sci. USA* **103**, 12301 – 12306 (2006).

63. “Principal component analysis of fast-folding λ-repressor mutants,” G. G. Maisuradze and D. M. Leitner, *Chem. Phys. Lett.* **421**, pp. 5 – 10 (2006).

62. “$CF_3CH_3 \rightarrow HF + CF_2CH_2$: A non-RRKM reaction?,” J. R. Barker, P. J. Stimac, K. D. King, and D. M. Leitner, *J. Phys. Chem. A* **110**, pp. 2944 – 2954 (2006).

61. “Thermal transport coefficients for liquid and glassy water computed from a harmonic aqueous glass,” X. Yu and D. M. Leitner, *J. Chem. Phys*. **123**, art. 104503, pp. 1-10 (2005).

60. “Influence of vibrational energy flow on isomerization of flexible molecules: incorporating non-RRKM kinetics in the simulation of dipeptide isomerization,” J. K. Agbo, D. M. Leitner, D. A. Evans and D. J. Wales, *J. Chem. Phys*. **123**, art. 124304, pp. 1-8 (2005).

59. “Mass fractal dimension and the compactness of proteins,” M. B. Enright and D. M. Leitner, *Phys. Rev. E* **71**, art. no. 011912, pp. 1-9 (2005).

58. “Heat flow in proteins: Computation of thermal transport coefficients,” X. Yu and D. M. Leitner, *J. Chem. Phys* **122**, art. no. 054902, pp. 1-11 (2005).

57. “Anharmonic decay of vibrational states in proteins,” X. Yu and D. M. Leitner, in *Normal mode analysis: Theory and applications to biological and chemical systems*; Q. Cui and I. Bahar, eds. (CRC Press, Boca Raton, 2005); pp. 325-348.

56. “Heat transport in molecules and reaction kinetics: the role of quantum energy flow and localization,” D. M. Leitner, *Advances in Chemical Physics* **130**, Part B, 205-256 (2005).

55. “Thermal transport in liquid and glassy water computed with normal modes,” X. Yu and D. M. Leitner, *Chem. Phys. Lett.* **398**, 480-485 (2004).

54. “Chromophore vibrations during isomerization of photoactive yellow protein: analysis of normal modes and energy transfer,” X. Yu and D. M. Leitner, *Chem. Phys. Lett*. **391**, 181 - 186 (2004).

53. “Anomalous diffusion of vibrational energy in proteins,” X. Yu and D. M. Leitner, *J. Chem. Phys.* **119**, 12673-12679 (2003).

52. “Thermodynamics of protein hydration computed by molecular dynamics and normal modes,” X. Yu, J. Park, and D. M. Leitner, *J. Phys. Chem. B* **107**, 12820 - 9 (2003).

51. “Quantum energy flow and trans-stilbene photoisomerization: an example of a non-RRKM reaction,” D. M. Leitner, B. Levine, J. Quenneville, T. J. Martinez, and P. G. Wolynes, *J. Phys. Chem. A* **107**, 10706 - 16 (2003).

50. “Vibrational energy transfer and heat conduction in a protein,” X. Yu and D. M. Leitner, *J. Phys. Chem. B* **107**, 1698 - 1707 (2003).

49. “Anharmonic decay of vibrational states in helical peptides, coils and one-dimensional glasses,” D. M. Leitner, *J. Phys. Chem. A* **106**, 10870 - 7 (2002). (R. S. Berry Festschrift)

48. “Temperature dependence of the pure vibrational dephasing rate in a heteropolymer,” D. M. Leitner, *Chem. Phys. Lett.* **359**, 434 – 439 (2002).

47. “Vibrational energy transfer in helices,” D. M. Leitner, *Phys. Rev. Lett*. **87**, art. no. 188102, pp. 1 - 4 (2001).

46. “Vibrational energy transfer and heat conduction in a one-dimensional glass,” D. M. Leitner, *Phys. Rev. B* **64**, art. no. 094201, pp. 1 - 9 (2001).

45. “Transient lattice dynamics in fs-laser-excited semiconductors probed by ultrafast x-ray diffraction,” K. Sokolowski-Tinten, M. H. von Hoegen, D. von der Linde, A. Cavalleri, C. W. Siders, F. L. H. Brown, D. M. Leitner, C. Toth, J. A. Squier, C. P. J. Barty, K. R. Wilson and M. Kammler, *Journal de Physique IV* **11**, 473 - 9 (2001).

44. “Anharmonic lattice dynamics in Germanium measured with ultrafast x-ray diffraction," A. Cavalleri, C. W. Siders, F. L. H. Brown, D. M. Leitner, C. Toth, J. A. Squier, C. P. J. Barty, K. R. Wilson, K. Sokolowski-Tinten, M. Horn von Hoegen, D. von der Linde and M. Kammler, *Phys. Rev. Lett.* **85**, 586 - 589 (2000).

43. "Lateral diffusion of membrane proteins in the presence of static and dynamic corrals: Suggestions for appropriate observables," F. L. H. Brown, D. M. Leitner, J. A. McCammon and K. R. Wilson, *Biophys. J*. **78**, 2257 - 67 (2000).

42. “Reduced density matrix approach to phononic dissipation in friction," A. Ozpineci, D. M. Leitner and S. Ciraci, *Phys. Rev. B* **62**, 10558 - 65 (2000).

41. "Heat flow through an insulating nanocrystal," D. M. Leitner and P. G. Wolynes, *Phys. Rev E* **61**, 2902 - 9 (2000).

40. "Regulation of protein mobility in cell membranes: A dynamic corral model," D. M. Leitner, F. L. H. Brown and K. R. Wilson, *Biophys. J.* **78**, 125 - 135 (2000).

39. "A model for phononic energy dissipation in friction," A. Buldum, D. M. Leitner and S. Ciraci, *Phys. Rev. B* **59**, 16042-9 (1999).

38. "Thermal conduction through a molecule," A. Buldum, D. M. Leitner and S. Ciraci, *Europhys. Lett*. **47**, 208-12 (1999).

37. "Influence of quantum energy flow and localization on molecular isomerization in gas and condensed phases," D. M. Leitner, *Int. J. Quantum Chem* **75**, 523-9 (1999).

36. "The vibrational energy flow transition in organic molecules: Theory meets experiment," R. Bigwood, M. Gruebele, D. M. Leitner and P. G. Wolynes, *Proc. Natl. Acad. Sci. USA* **95**, 5960-7 (1998).

35. "Mesoscopic motion of atomic ions in magnetic fields," D. M. Leitner and P. Schmelcher, *Phys. Rev. A* **58**, R3383-6 (1998).

34. "Quantum energy flow during molecular isomerization," D. M. Leitner and P. G. Wolynes, *Chem. Phys. Lett.* **280**, 411-8 (1997).

33. "Effects of symmetry breaking on statistical properties of near-lying acoustic resonances," D. M. Leitner, *Phys. Rev. E* **56**, 4890-2 (1997).

32. "Predictions of local random matrix theory for vibrational mixing and energy flow in polyatomics," D. M. Leitner and P. G. Wolynes, *ACH Models in Chemistry* **134**, 663 (1997) (Special issue: "Dynamical Information from Molecular Spectra by Statistical Methods").

31. "Comment on: 'Level dynamics under magnetic field: a tool for statistical studies of rovibronic interactions in the NO_2 molecule'," D. M. Leitner and P. G. Wolynes, *ACH Models in Chemistry* **134**, 569 (1997).

30. "Comment on: 'A time dependent view of the statistics of spectral intensities'," D. M. Leitner and P. G. Wolynes, *ACH Models in Chemistry* **134**, 612 (1997).

29. "Comment on: 'Dynamic bottlenecks and the extreme stability of high Rydberg states'," D. M. Leitner and P. G. Wolynes, *ACH Models in Chemistry* **134**, 634 (1997).

28. "Comment on: 'Models of intramolecular energy redistribution'," D. M. Leitner and P. G. Wolynes, *ACH Models in Chemistry* **134**, 658 (1997).

27. "Quantization of the stochastic pump model of Arnold diffusion," D. M. Leitner and P. G. Wolynes, *Phys. Rev. Lett.* **79**, 55 - 58 (1997).

26. "Intramolecular energy flow in the condensed phase: Effects of dephasing on localization in the quantum stochastic pump model," D. M. Leitner and P. G. Wolynes, *Chem. Phys. Lett*. **276**, 289-95 (1997).

25. "The effects of three-body (Axelrod-Teller) forces on the classical and quantum behavior of rare gas trimers," C. Chakravarty, R. J. Hinde, D. M. Leitner and D. J. Wales, *Phys. Rev. E* **56**, 363-73 (1997).

24. "Vibrational mixing and energy flow in polyatomics: Quantitative prediction using local random matrix theory," D. M. Leitner and P. G. Wolynes, *J. Phys. Chem*. **101**, 541 (1997) (Saburo Nagakura Festschrift).

23. "Statistical properties of localized vibrational eigenstates," D. M. Leitner and P. G. Wolynes, *Chem. Phys. Lett*. **258**, 18 (1996).

22. "Vibrational relaxation and energy localization in polyatomics: Effects of high-order resonances on flow rates and the quantum ergodicity transition," D. M. Leitner and P. G. Wolynes, *J. Chem. Phys*. **105**, 11226 - 11236 (1996).

21. "Many-dimensional energy flow at low energy," D. M. Leitner and P. G. Wolynes, *Phys. Rev. Lett*. **76**, 216 - 219 (1996).

20. "Statistical properties of molecular spectra and molecular dynamics: analysis of their correspondence in NO_2 and $C_2H_4^+$," D. M. Leitner, H. Köppel, and L. S. Cederbaum, *J. Chem. Phys*. **104**, 434 - 443 (1996).

19. "Semiclassical localization in time-independent K-systems," M. Feingold and D. M. Leitner, in Nonlinear Phenomena and Mesoscopic Systems, G. Casati, H. Cerdeira and S. Lundqvist, Eds. (World Scientific, 1995).

18. "Effects of symmetry breaking on spectra of chaotic Hamiltonian systems," D. M. Leitner, H. Köppel, and L. S. Cederbaum, *Phys. Rev. Lett*. **73**, 2970 - 3 (1994).

17. "Some properties of invariant random matrix ensembles and their connection to ergodic and nonergodic Hamiltonian systems," D. M. Leitner and L. S. Cederbaum, *Phys. Rev. E* **49**, 114 (1994).

16. "Real-symmetric random matrix ensembles of Hamiltonians with partial symmetry-breaking," D. M. Leitner, *Phys. Rev. E* **48**, 2536 - 46 (1993).

15. "Invariant random matrix ensembles as models for ergodic and nonergodic Hamiltonian systems," D. M. Leitner and L. S. Cederbaum, *J. Mol. Struct.* **292**, 197 (1993).

14. "Density of states of band random matrices with electric field," D. M. Leitner and M. Feingold, *J. Phys. A* **26**, 7367 (1993).

13. "Vibrational states of Lennard-Jones trimers," D. M. Leitner, J. D. Doll, and R. M. Whitnell, *J. Chem. Phys*. **96**, 9239 (1992).

12. Book Review: Algorithms for Chemists, D. M. Leitner, *J. Am. Chem. Soc*. 114, 1931 (1992).

11. "The quantum mechanics of clusters: the low temperature equilibrium and dynamical behavior of rare gas systems," S. W. Rick, D. M. Leitner, J. D. Doll, D. L. Freeman, and D. D. Frantz, *J. Chem. Phys*. **95**, 6658 (1991).

10. "Localization and spectral statistics in a banded random matrix ensemble," M. Wilkinson, M. Feingold, and D. M. Leitner, *J. Phys. A* **24**, 175 (1991).

9. "Spectral statistics in semiclassical random matrix ensembles," M. Feingold, D. M. Leitner, and M. Wilkinson, *Phys. Rev. Lett*. **66**, 986 (1991).

8. "Variational calculation of the rovibrational spectrum of H_2O using the coupled-rotor basis," D. M. Leitner, J. E. Hunter III, G. A. Natanson, R. S. Berry, P. Villarreal, and G. Delgado-Barrio, *J. Chem. Phys.* **94**, 5917 (1991).

7. "Quantum mechanics of small Ne, Ar, Kr, and Xe clusters," D. M. Leitner, J. D. Doll, and R. M. Whitnell, *J. Chem. Phys.* **94**, 6644 (1991).

6. "Semiclassical structure of Hamiltonians," M. Feingold, D. M. Leitner, and O. Piro, *Phys. Rev. A* **39**, 6507 (1989).

5. "Quantum chaos of Ar_3: statistics of eigenvalues," D. M. Leitner, R. S. Berry, and R. M. Whitnell, *J. Chem. Phys*. **91**, 3470 (1989).

4. "Melting and phase space transitions in small clusters: spectral characteristics, dimensions, and K-entropy," T. L. Beck, D. M. Leitner, and R. S. Berry*, J. Chem. Phys*. **89**, 1681 (1988).

3. "Particles-on-a-sphere method for computing the rotational-vibrational spectrum of H_2O," D. M. Leitner, G. A. Natanson, R. S. Berry, P. Villarreal, and G. Delgado-Barrio, *Comp. Phys. Comm*. **51**, 207 (1988).

2. "Diode laser spectroscopy of the ν_2 band of CD_3," J. M. Frye, T. J. Sears, and D. M. Leitner, *J. Chem. Phys.* **88**, 5300 - 5306 (1988).

1. "Theoretical intensities for rotation-vibration lines of water using particles-on-a-sphere wavefunctions," J. E. Hunter III, D. M. Leitner, G. A. Natanson, and R. S. Berry, *Chem. Phys. Lett.* **144**, 145 (1988).