

## Curriculum Vitae

David M. Leitner  
Department of Chemistry and Chemical Physics Program  
University of Nevada, Reno/216  
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### 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:

- 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:

- 2019            Japan Society for the Promotion of Science (JSPS) Invitational Fellow  
2018            Appointed to Editorial Advisory Board of *Journal of Physical Chemistry*  
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  
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 (Sept. – Dec.)	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 the Physics of Complex Systems, Dresden

### **Grants Awarded:**

06.15.14 – 05.31.19	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.)*

132. Plenary speaker, XXXIX. Dynamics Days Europe Conference, Rostock, Germany, Sept. 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, Oct. 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, Jan. 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. Pacificchem 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. 7<sup>th</sup> US-Japan Joint Seminar on Nanoscale Transport Phenomena, Shima, Japan, Dec. 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. Pacificchem Symposium on Spectr. Probes of Intermolecular Interactions, 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, Jul. 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. 6<sup>th</sup> Congress of International Society for Theor. Chem. Phys., U. British Columbia, July 08.
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, Jan. 08.
59. Workshop on Computational Biophysics, Nagoya University, Nagoya, Japan, Nov. 2007.
58. Telluride Workshop on Vibrational Dynamics, Telluride Science Research Center, Aug. 07.
57. Physical Chemistry Institute, Universität Heidelberg, Heidelberg, Germany, May 2007.
56. Bunsen Discussion Meeting, "Exploring THz Spectroscopy", Bad Honnef, Germany, Apr. 07
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, Dec. 06.
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, Aug. 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, Nov. 1999.
12. Department of Chemistry, Cambridge University, Cambridge, England, Oct. 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:**

10. Pacificchem Symposium, “Biomolecules at interfaces defining the cellular environment: From conformational dynamics to informatics approaches,” Pacificchem 2020, Honolulu, Hawaii (with Masataka Nagaoka, Nagoya U.; John Straub, BU; Changbong Hyeon, Korea Institute for Advanced Study (KIAS)).
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. Pacificchem Symposium, “Conformational dynamics of biomolecules and the biomolecule-solvent interface,” Pacificchem 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,” Physikzentrum, 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* (2): Matt Enright, Mia Swain.

*Undergraduates* (10): Reya Kempley, David Ponte, Chantal Reyna, Patrick Tomco, Ben Borgo, Amber Jain, Taylor Kaplan, Marcus Sacchetti, Marie Jones, James Ludwig.

*Graduate Students* (6): Johnson Agbo, Yao Xu, Hari Pandey, Korey Reid, David Kirkland, Humanath Poudel.

*Postdoctoral Associates* (4): Xin Yu, Gia Maisuradze, J. Park, Ramachandran Gnanasekaran.

## **Courses Taught:**

CHEM 121, General Chemistry 1 (Spring 2005, Spring 2010)

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, 2010, 2011, 2012, 2017)

CHEM 655, (Boston University) Statistical Mechanics (Spring 2012)

CHEM 751, Non-Equilibrium Statistical Mechanics (Spring 2009)

CHEM 754, Molecular Spectroscopy (Spring 2002, Fall 2005, 2009, 2013, 2015)

CHEM 755, Statistical Thermodynamics (Spring 2004, 2006, 2008, 2016, 2018)

CHEM 757, Quantum Chemistry (Fall 2000, 2002, 2008, 2010, 2014, 2016, 2018)

\* 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 – 2020)

Director, Chemical Physics Program (2009 – 2017)

Center for Advanced Studies, Member (2014 – present), Executive Committee (2016 – 18)

UNR Outstanding Researcher Award Committee, Member (2015 – 2019), Chair (2018)

UNR Selection Committee for Nevada Regents' Outstanding Researcher Award (2016 - 17)

Mousel-Feltner Award Committee (2005, 2006, 2008, 2010; Chair, 2006, 2010)

Shin Award Committee (Chair, 2012)

College of Science Personnel Committee (2009 – 12)

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 Department Theory Search Committee, Member (2003 - 2004)

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 Secretary/Treasurer (2010 – 2013)

*The Journal of Chemical Physics*

Editorial Advisory Board (2016 – 2018)

*Scientific Reports - Nature*

Editorial Board (2017 – 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 – present)

*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*, *Physical Review 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 and Francis Publ.; *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); Agence Nationale de la Recherche (France); Israel Science Foundation; National Science Centre, Poland; Austrian Science Fund, Freiburg Institute for Advanced Studies (FRIAS).

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

*National Science Foundation panelist*

CRIF (2005); Theo. & Comp. Chemistry (2008, 2015, 2016); Chem. of Life Processes (2017)

**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:

120. "Molecules and the Eigenstate Thermalization Hypothesis," *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.jpccb.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**, pp. 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**, pp. 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**, pp. 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).
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