David M Leitner

List of Publications by Year in Descending Order

113 papers	4,230 citations	38 h-index	62 g-index
119 ext. papers	4,574 ext. citations	4.2 avg, IF	5.98 L-index

#	Paper	IF	Citations
113	The origin and impact of bound water around intrinsically disordered proteins.. *Biophysical Journal*, **2022**,	2.9	3
112	Richard Stephen Berry (1931–2020) **2022**, 27, 11-17		
111	Enhanced Mobility during Diels-Alder Reaction: Results of Molecular Simulations.. *Journal of Physical Chemistry Letters*, **2022**, 3763-3769	6.4	0
110	Locating and Navigating Energy Transport Networks in Proteins. *Methods in Molecular Biology*, **2021**, 2253, 37-59	1.4	
109	Activation-Induced Reorganization of Energy Transport Networks in the β-Adrenergic Receptor. *Journal of Physical Chemistry B*, **2021**, 125, 6522-6531	3.4	2
108	Change in vibrational entropy with change in protein volume estimated with mode Grüneisen parameters. *Journal of Chemical Physics*, **2021**, 154, 055102	3.9	6
107	Electric Fields Influence Intramolecular Vibrational Energy Relaxation and Line Widths. *Journal of Physical Chemistry Letters*, **2021**, 12, 7818-7825	6.4	2
106	Network models of biological adaptation at the molecular scale: Comment on "Dynamic and thermodynamic models of adaptation" by A.N. Gorban et al. *Physics of Life Reviews*, **2021**, 38, 124-126	2.1	2
105	Water-mediated biomolecular dynamics and allostery. *Journal of Chemical Physics*, **2020**, 152, 240901	3.9	11
104	Structure, dynamics, and energy flow that govern Heme protein functions: theory and experiments. Session 3SBA at the 57th BSJ Annual Meeting. *Biophysical Reviews*, **2020**, 12, 291-292	3.7	0
103	Recent developments in the computational study of protein structural and vibrational energy dynamics. *Biophysical Reviews*, **2020**, 12, 317-322	3.7	8
102	Energy Relaxation and Thermal Transport in Molecules **2020**, 865-885		
101	Variation of Energy Transfer Rates across Protein-Water Contacts with Equilibrium Structural Fluctuations of a Homodimeric Hemoglobin. *Journal of Physical Chemistry B*, **2020**, 124, 1148-1159	3.4	9
100	Energy Transfer across Nonpolar and Polar Contacts in Proteins: Role of Contact Fluctuations. *Journal of Physical Chemistry B*, **2020**, 124, 9852-9861	3.4	6
99	Energy Transport across Interfaces in Biomolecular Systems. *Journal of Physical Chemistry B*, **2019**, 123, 9507-9524	3.4	21
98	Illuminating Fermi Resonances that Trigger Reaction in a Complex Molecule. *CheM*, **2019**, 5, 256-257	16.2	3
97	Elastic and Inelastic Contributions to Thermal Transport between Chemical Groups and Thermal Rectification in Molecules. *Journal of Physical Chemistry C*, **2019**, 123, 6256-6264	3.8	10

96	Tuning Molecular Vibrational Energy Flow within an Aromatic Scaffold via Anharmonic Coupling. *Journal of Physical Chemistry A*, **2019**, 123, 10571-10581	2.8	10
95	Energy Relaxation and Thermal Transport in Molecules **2018**, 1-22		
94	Vibrational States and Nitrile Lifetimes of Cyanophenylalanine Isotopomers in Solution. *Journal of Physical Chemistry A*, **2018**, 122, 6856-6863	2.8	5
93	MAPPING ENERGY TRANSPORT NETWORKS IN PROTEINS. *Reviews in Computational Chemistry*, **2018**, 63-113		5
92	Molecules and the Eigenstate Thermalization Hypothesis. *Entropy*, **2018**, 20,	2.8	8
91	Scaling of Rates of Vibrational Energy Transfer in Proteins with Equilibrium Dynamics and Entropy. *Journal of Physical Chemistry B*, **2018**, 122, 9331-9339	3.4	20
90	Hydrophobic Collapse of Ubiquitin Generates Rapid Protein-Water Motions. *Biochemistry*, **2018**, 57, 3650-3657	3.2	9
89	Small Saccharides as a Blanket around Proteins: A Computational Study. *Journal of Physical Chemistry B*, **2018**, 122, 7277-7285	3.4	9
88	Influence of thermalization on thermal conduction through molecular junctions: Computational study of PEG oligomers. *Journal of Chemical Physics*, **2017**, 147, 084701	3.9	28
87	Thermodynamics of Hydration Water around an Antifreeze Protein: A Molecular Simulation Study. *Journal of Physical Chemistry B*, **2017**, 121, 9498-9507	3.4	16
86	Vibrational energy transport in molecules and the statistical properties of vibrational modes. *Chemical Physics*, **2017**, 482, 81-85	2.3	15
85	Thermalization and Thermal Transport in Molecules. *Journal of Physical Chemistry Letters*, **2016**, 7, 5062-5067	5.1	30
84	Scaling Rules for Vibrational Energy Transport in Globular Proteins. *Journal of Physical Chemistry Letters*, **2016**, 7, 25-30	6.4	42
83	Hydrophobic collapse induces changes in the collective protein and hydration low frequency modes. *Chemical Physics Letters*, **2016**, 651, 1-7	2.5	13
82	Protein□water dynamics in antifreeze protein III activity. *Chemical Physics Letters*, **2016**, 647, 1-6	2.5	25
81	Water-Mediated Energy Dynamics in a Homodimeric Hemoglobin. *Journal of Physical Chemistry B*, **2016**, 120, 4019-27	3.4	15
80	Quantum ergodicity and energy flow in molecules. *Advances in Physics*, **2015**, 64, 445-517	18.4	70
79	Size-Dependent Accuracy of Nanoscale Thermometers. *Journal of Physical Chemistry B*, **2015**, 119, 9000-5	3.4	15

78	Quantum bottlenecks and unidirectional energy flow in molecules. *Annalen Der Physik*, **2015**, 527, 601-609	2.6	14
77	Vibrational energy flow in the villin headpiece subdomain: master equation simulations. *Journal of Chemical Physics*, **2015**, 142, 075101	3.9	42
76	Asymmetric energy flow in liquid alkylbenzenes: A computational study. *Journal of Chemical Physics* , **2015**, 143, 144301	3.9	18
75	The role of sulfates on antifreeze protein activity. *Journal of Physical Chemistry B*, **2014**, 118, 7920-4	3.4	24
74	Vibrational energy flow through the green fluorescent protein-water interface: communication maps and thermal boundary conductance. *Journal of Physical Chemistry B*, **2014**, 118, 7818-26	3.4	36
73	Communication maps of vibrational energy transport through Photoactive Yellow Protein. *Journal of Physical Chemistry A*, **2014**, 118, 7280-7	2.8	14
72	Vibrational energy flow across heme□ytochrome c and cytochrome c□water interfaces. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	23
71	Thermal Conductance at the Interface Between Molecules. *Advances in Chemical Physics*, **2014**, 159-163		
70	Communication Maps: Exploring Energy Transport through Proteins and Water. *Israel Journal of Chemistry*, **2014**, 54, 1065-1073	3.4	13
69	The dielectric response to photoexcitation of GFP: A molecular dynamics study. *Chemical Physics Letters*, **2013**, 564, 78-82	2.5	14
68	Long-range protein-water dynamics in hyperactive insect antifreeze proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 1617-22	11.5	192
67	Thermal boundary conductance and thermal rectification in molecules. *Journal of Physical Chemistry B*, **2013**, 117, 12820-8	3.4	64
66	Mode damping rates in a protein chromophore. *Chemical Physics Letters*, **2012**, 530, 102-106	2.5	17
65	Analysis of Water and Hydrogen Bond Dynamics at the Surface of an Antifreeze Protein. *Journal of Atomic, Molecular, and Optical Physics*, **2012**, 2012, 1-6		11
64	THz Technology and THz Spectroscopy: Modeling and Experiments to Study Solvation Dynamics of Biomolecules **2012**, 687-710		
63	Protein Functional Motions: Basic Concepts and Computational Methodologies. *Advances in Chemical Physics*, **2011**, 35-82		7
62	Ergodic Problems for Real Complex Systems in Chemical Physics. *Advances in Chemical Physics*, **2011** , 171-220		4
61	Non-Brownian Phase Space Dynamics of Molecules, the Nature of their Vibrational States, and Non-RRKM Kinetics. *Advances in Chemical Physics*, **2011**, 83-122		5

60	Dynamical Reaction Theory based on Geometric Structures in Phase Space. *Advances in Chemical Physics*, **2011**, 123-169		5
59	Dielectric response and vibrational energy relaxation in photoactive yellow protein: A molecular dynamics simulation study. *Chemical Physics Letters*, **2011**, 516, 102-105	2.5	6
58	Communication maps computed for homodimeric hemoglobin: computational study of water-mediated energy transport in proteins. *Journal of Chemical Physics*, **2011**, 135, 065103	3.9	45
57	Non-Markovian Theory of Vibrational Energy Relaxation and its Applications to Biomolecular Systems. *Advances in Chemical Physics*, **2011**, 1-33		6
56	Quantum localization and protein-assisted vibrational energy flow in cofactors. *New Journal of Physics*, **2010**, 12, 085004	2.9	23
55	Dynamics of water clusters confined in proteins: a molecular dynamics simulation study of interfacial waters in a dimeric hemoglobin. *Journal of Physical Chemistry B*, **2010**, 114, 16989-96	3.4	55
54	Quantum localization, dephasing and vibrational energy flow in a trans-formanilide (TFA)H2O complex. *Chemical Physics*, **2010**, 374, 111-117	2.3	3
53	Frequency-resolved communication maps for proteins and other nanoscale materials. *Journal of Chemical Physics*, **2009**, 130, 195101	3.9	66
52	Rattling in the cage: ions as probes of sub-picosecond water network dynamics. *Journal of the American Chemical Society*, **2009**, 131, 18512-7	16.4	116
51	A quantum model of restricted vibrational energy flow on the way to the transition state in unimolecular reactions. *Molecular Physics*, **2008**, 106, 433-442	1.7	46
50	Solvation dynamics of biomolecules: modeling and terahertz experiments. *HFSP Journal*, **2008**, 2, 314-23		98
49	Energy flow in proteins. *Annual Review of Physical Chemistry*, **2008**, 59, 233-59	15.7	234
48	Protein sequence- and pH-dependent hydration probed by terahertz spectroscopy. *Journal of the American Chemical Society*, **2008**, 130, 2374-5	16.4	111
47	Free energy landscape of a biomolecule in dihedral principal component space: sampling convergence and correspondence between structures and minima. *Proteins: Structure, Function and Bioinformatics*, **2007**, 67, 569-78	4.2	78
46	Quantum energy flow and the kinetics of water shuttling between hydrogen bonding sites on trans-formanilide. *Journal of Chemical Physics*, **2007**, 127, 064315	3.9	15
45	An extended dynamical hydration shell around proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 20749-52	11.5	512
44	Biomolecule large-amplitude motion and solvation dynamics: modelling and probes from THz to X-rays. *International Reviews in Physical Chemistry*, **2006**, 25, 553-582	7	73
43	Hydration dependence of the mass fractal dimension and anomalous diffusion of vibrational energy in proteins. *Physical Review E*, **2006**, 73, 051905	2.4	23

42	Thermal conductivity computed for vitreous silica and methyl-doped silica above the plateau. *Physical Review B*, **2006**, 74,	3.3	16
41	CF3CH3 --> HF + CF2CH2: a non-RRKM reaction?. *Journal of Physical Chemistry A*, **2006**, 110, 2944-54	2.8	20
40	Quantum theory of enhanced unimolecular reaction rates below the ergodicity threshold. *Chemical Physics*, **2006**, 329, 163-167	2.3	28
39	Mass fractal dimension and the compactness of proteins. *Physical Review E*, **2005**, 71, 011912	2.4	93
38	1SD05 Vibrational dynamics and energy transport in proteins. *Seibutsu Butsuri*, **2005**, 45, S6	0	
37	Heat Transport in Molecules and Reaction Kinetics: The Role of Quantum Energy Flow and Localization. *Advances in Chemical Physics*, **2005**, 205-256		37
36	Heat flow in proteins: computation of thermal transport coefficients. *Journal of Chemical Physics*, **2005**, 122, 54902	3.9	85
35	Thermal transport coefficients for liquid and glassy water computed from a harmonic aqueous glass. *Journal of Chemical Physics*, **2005**, 123, 104503	3.9	14
34	Influence of vibrational energy flow on isomerization of flexible molecules: incorporating non-Rice-Ramsperger-Kassel-Marcus kinetics in the simulation of dipeptide isomerization. *Journal of Chemical Physics*, **2005**, 123, 124304	3.9	24
33	Chromophore vibrations during isomerization of photoactive yellow protein: analysis of normal modes and energy transfer. *Chemical Physics Letters*, **2004**, 391, 181-186	2.5	10
32	Thermal transport in liquid and glassy water computed with normal modes. *Chemical Physics Letters* , **2004**, 398, 480-485	2.5	8
31	Quantum Energy Flow and trans-Stilbene Photoisomerization: an Example of a Non-RRKM Reaction *Journal of Physical Chemistry A*, **2003**, 107, 10706-10716	2.8	88
30	Thermodynamics of Protein Hydration Computed by Molecular Dynamics and Normal Modes. *Journal of Physical Chemistry B*, **2003**, 107, 12820-12828	3.4	38
29	Vibrational Energy Transfer and Heat Conduction in a Protein. *Journal of Physical Chemistry B*, **2003**, 107, 1698-1707	3.4	141
28	Anomalous diffusion of vibrational energy in proteins. *Journal of Chemical Physics*, **2003**, 119, 12673-12679	3.9	71
27	Temperature dependence of the pure vibrational dephasing rate in a heteropolymer. *Chemical Physics Letters*, **2002**, 359, 434-439	2.5	7
26	Anharmonic Decay of Vibrational States in Helical Peptides, Coils, and One-Dimensional Glasses *Journal of Physical Chemistry A*, **2002**, 106, 10870-10876	2.8	22
25	Vibrational Energy Transfer in Helices. *Physical Review Letters*, **2001**, 87,	7.4	63

24	Vibrational energy transfer and heat conduction in a one-dimensional glass. *Physical Review B*, **2001**, 64,	3.3	53
23	Heat flow through an insulating nanocrystal. *Physical Review E*, **2000**, 61, 2902-2908	2.4	38
22	Influence of quantum energy flow and localization on molecular isomerization in gas and condensed phases. *International Journal of Quantum Chemistry*, **1999**, 75, 523-531	2.1	39
21	Mesoscopic motion of atomic ions in magnetic fields. *Physical Review A*, **1998**, 58, R3383-R3386	2.6	3
20	Effects of three-body (Axilrod-Teller) forces on the classical and quantum behavior of rare-gas trimers. *Physical Review E*, **1997**, 56, 363-377	2.4	30
19	Effects of symmetry breaking on statistical properties of near-lying acoustic resonances. *Physical Review E*, **1997**, 56, 4890-4891	2.4	13
18	Quantization of the Stochastic Pump Model of Arnold Diffusion. *Physical Review Letters*, **1997**, 79, 55-58	7.4	42
17	Vibrational Mixing and Energy Flow in Polyatomics: Quantitative Prediction Using Local Random Matrix Theory. *Journal of Physical Chemistry A*, **1997**, 101, 541-548	2.8	59
16	Intramolecular energy flow in the condensed phase: effects of dephasing on localization in the quantum stochastic pump model. *Chemical Physics Letters*, **1997**, 276, 289-295	2.5	12
15	Quantum energy flow during molecular isomerization. *Chemical Physics Letters*, **1997**, 280, 411-418	2.5	78
14	Statistical properties of localized vibrational eigenstates. *Chemical Physics Letters*, **1996**, 258, 18-24	2.5	47
13	Many-dimensional quantum energy flow at low energy. *Physical Review Letters*, **1996**, 76, 216-219	7.4	51
12	Statistical properties of molecular spectra and molecular dynamics: Analysis of their correspondence in NO2 and C2H+4. *Journal of Chemical Physics*, **1996**, 104, 434-443	3.9	46
11	Vibrational relaxation and energy localization in polyatomics: Effects of high-order resonances on flow rates and the quantum ergodicity transition. *Journal of Chemical Physics*, **1996**, 105, 11226-11236	3.9	58
10	Some properties of invariant random-matrix ensembles and their connection to ergodic and nonergodic Hamiltonian systems. *Physical Review E*, **1994**, 49, 114-121	2.4	6
9	Effects of symmetry breaking on spectra of chaotic Hamiltonian systems. *Physical Review Letters*, **1994**, 73, 2970-2973	7.4	37
8	Real symmetric random matrix ensembles of Hamiltonians with partial symmetry breaking. *Physical Review E*, **1993**, 48, 2536-2546	2.4	46
7	Vibrational states of Lennard-Jones trimers. *Journal of Chemical Physics*, **1992**, 96, 9239-9240	3.9	6

6	Quantum mechanics of small Ne, Ar, Kr, and Xe clusters. *Journal of Chemical Physics*, **1991**, 94, 6644-6659	3.9	68
5	Spectral statistics in semiclassical random-matrix ensembles. *Physical Review Letters*, **1991**, 66, 986-989	7.4	70
4	Quantum chaos of Ar3: Statistics of eigenvalues. *Journal of Chemical Physics*, **1989**, 91, 3470-3476	3.9	58
3	Semiclassical structure of Hamiltonians. *Physical Review A*, **1989**, 39, 6507-6514	2.6	46
2	Melting and phase space transitions in small clusters: Spectral characteristics, dimensions, and K entropy. *Journal of Chemical Physics*, **1988**, 89, 1681-1694	3.9	97
1	Diode laser spectroscopy of the 2 band of CD3. *Journal of Chemical Physics*, **1988**, 88, 5300-5306	3.9	30