CURRICULUM VITAE

DAVE THIRUMALAI

Collie-Welch Reagents Professor in Chemistry

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http://scholar.google.com/citations?user=sNiAY9IAAAAJ&hl=en (H-index – 96; Citations-31,657
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FIELD OF SPECIALIZATION

Theoretical and Computational Chemistry

EDUCATIONAL BACKGROUND

1972-1977: **M.Sc. (First Class)** Indian Institute of Technology, Kanpur, India
(50% courses in basic engineering)
Undergraduate Thesis: "The E.S.R. Spectra of Some Aromatic Nitro Compounds"

1977-1982: **Ph.D.** Candidate in Physical Chemistry, University of Minnesota
Research Advisor: **Professor Donald G. Truhlar**
Graduate Thesis Title: "Effective Potential Studies of Electron-Atom and Electron-Molecule Collisions"

PROFESSIONAL EXPERIENCE

1982-1985: Postdoctoral Research Associate, Columbia University, New York
Research Advisor: **Professor Bruce J. Berne**

1985-1989: Assistant Professor, University of Maryland

1989-1993: Associate Professor, University of Maryland

1993- 2010 Professor, University of Maryland

1990-2005: Guest Worker, National Institute for Standards and Technology, Gaithersburg, MD

July 1995 Visiting Professor, Service de Physique Theorique, Saclay, France

March-June 1996 Forcheimer Professor, Hebrew University, Jerusalem, Israel

October 1998-
January 1999 Fellow, Institute for Advanced Study, Hebrew University, Jerusalem

2005-2011 Founding Director, Biophysics Program, University of Maryland
October 2009 Oden Fellow, University of Texas, Austin
Aug-Sep (2012) Oden Fellow, University of Texas, Austin
Aug 2011-Jul 2013 Visiting Professor, Biophysics Department, Nanjing, China
Jan 2011-Dec 2013 Visiting Scholar, Korea Institute for Advanced Studies, Seoul, Korea
2010- 2015 **Distinguished University Professor**, University of Maryland
2016 - present **Collie-Welch Reagents Chair,** University of Texas at Austin
2018-2020 **Weston Visiting Professorship,** Weizmann Institute, Rehovat Israel
2015-2019 Advisory Committee, Simons Center for Study of Living Systems, NCBS Bangalore

Awards

National Science Talent Research Fellow, India	1972-1977
Camille and Henry Dreyfus Foundation: Distinguished New Faculty Award	1985-1987
Alfred P. Sloan Fellowship	1986-1988
Presidential Young Investigator Award	1987-1992
Outstanding Junior Faculty Award, University of Maryland	1989
Camille and Henry Dreyfus Foundation, Teacher Scholar Award	1990
Maryland Outstanding Young Scientist	1995
Distinguished Faculty Research Fellowship Award, University of Maryland	1998
Humboldt Research Award for Senior U.S. Scientists	2009
Elected to Royal Society of Chemistry	2009
Honorary Senior Hans-Fisher Fellow, Technical University of Munich	2011
Elected Fellow Biophysical Society	2014
Chemical Research Society of India (CRSI) Medal	2016
Elected Fellow American Physical Society	2016
ACS Theoretical Chemistry Award (Physical Chemistry Division)	2016
Oesper Award, Chemistry, University of Cincinnati	2018
APS Award, Irving Langmuir Prize	2019
Hans Neurath Award, Protein Society	2019

Professional Service

Co-Organizer International meeting on “Protein folding and Dynamics,” NCBS Bangalore, Oct 15-17 (2012).
Chair 2012 Gordon Research Conference “Protein folding and Dynamics” January 8-13, 2012.
Chair NSF Workshop on “RNA and Protein Folding and beyond: A vision for the next decade”, September 12 and 13, 2011.
Chair External Review Committee (NSF) Center for Theoretical and Biological Physics, 2011
Advisory Board NIH Resource Center, UIUC (Chair 2010). Member 2008, 2009, and 2011.
Vice Chair (elected) for 2010 Gordon Research Conference "Protein Folding and Dynamics"
Co-Organizer International meeting on “Protein folding and Dynamics,” NCBS Bangalore, Nov 5-7 (2014).

Editorial Services

PMC Biophysics (2008-2010)

BMC Biophysics (2011-present)
Protein Engineering Design and Selection (2004-present)
Editorial Board F1000 (2010-present).
Editorial Board J. Statistical Physics (2013-2015).
Journal of Chemical Physics (2008-2010).
Associate Editor: Communications in Mathematical Sciences (2003-2005).
Editorial Board: Theoretical Chemistry Accounts (1997-2004).
Editorial Board: J. Physical Chemistry (2015-2017).
Editorial Board: Biology Direct

Panel Member: NSF Postdoctoral Fellowship in Computations (1997).
Panel Member: NSF Career Awards (1997, 2008)
Panel Member: Special Emphasis Panel on Material Theory Programs chaired by Prof. J.R. Schrieffer (1997)

Special Lectures

1) A mini course (10 lectures) on Folding of Biomolecules, Institute for Theoretical Physics, Santa Barbara, CA, July 1997.

2) Key Note Speaker, GRC meeting "Protein Folding and Dynamics", CA 2008.

3) Key Note Address: Student Sponsored Symposium Molecular Genetics & Cell Biology, University of Chicago, May 2008.

4) Zhonsong Distinguished Lecturer in Biophysics, Nanjing University, China, December 12, 2008.

5) IBSI Distinguished Scientific Leader Lecture, Georgia Tech University, May 11, 2011

6) Mini course (3 three hour lectures) on "A primer in Single Molecule Force Spectroscopy" EPFL, Lausanne, Switzerland, October 6, 13, and 20 2011.

7) Tenneco Lectureship, Department of Physics, University of Houston, April 25, 2012

8) Keynote Speaker, "International Conference on Molecular Crowding", June 12, 2012, Monte Verita, Locarno, Switzerland.

9) Summer School on Active Systems, GIST, Gwangju, Korea Four lectures, June 24 – June 26 2014.

10) The 3rd Soft Matter Summer School: Polymers in Biology, June 29 and July 1, 2015, Korea Institute for Advanced Studies, Seoul, Korea.

11) Lecturer Summer School, Madrid, July 2016.
12) Plenary Speaker Third International Conference on Computational Science and Engineering, Hoh Chi Minh City, Vietnam, November 2016.

13) Plenary Speaker, Texas Folders & Function Meeting, Cleveland, TX, April, 2017

GRADUATE STUDENTS (and their subsequent positions)

***Previous graduate students*:**

Zhuyan Guo; Senior Research Scientist, Merck;
M. Molisana, Professor, Lesotho;
M.R. Shaw, Institute for Defense Analysis;
Changbong Hyeon, Professor Dept. of Computational Sciences, Korea Institute for Advanced Studies;
Bae-Yun Ha, Professor, Department of Physics, Waterloo Univ.

Greg Morrison, Assistant Professor, Physics Department, University of Houston;
Edward P. O'Brien, Associate Professor, Department of Chemistry, Penn State University;
Jie Chen, Postdoctoral Scholar, Columbia University;
Biyun Shi;
Zhechun (Lance) Zhang Postdoctoral Fellow, Harvard University;

Guy Ziv (Part time) Professor, University of Leeds, UK
Daniel Lidar (Part time) Professor, USC, CA
Shaon Chakraborty Postdoctoral Fellow, Harvard University Medical School
Hongsuk Kang Postdoctoral Fellow, IBM Yorktown Heights, NY
Houng Vu (Postdoctoral Fellow in Warwick University)

Yonathan Cwik (EMBO Fellow, LMU Cambridge, UK)

***Current graduate students**:*

Guang Shi, Sumit Sinha, Atreya Dey, Davin Jeong, Ryota Takai

Current Postdoctoral Fellows:

Himadri Samanta, Naoto Hori, Mauro Mugnai, Xin Li, Abdul Nasser, Marina Katava, Sabeeha Hasnan, Hung T. Nguyen, Debyan Chakaborty, Hyun Woo Cho, Sucheol Shin

POSTDOCTORAL ASSOCIATES and FELLOWS (and subsequent positions)

***Previous associates**:*

J. Dana Honeycutt, Research Scientist, Corning, San Diego
Robert Rosenberg, Naval Research Laboratory
Carlos A. Condat, Professor, Physics, National University of Cordoba, Cordoba, Argentina
David Pincus, Graduate Student in Mathematics, University of Maryland
Sarvin Moghaddam

Vladimir Dobrosavljevic, Professor, Department of Physics, Florida State Univ.;

Harmen Bussemaker, Professor, Department of Biology, Columbia Univ.;
Carlos J. Camacho, Professor, Department of Computational Biology, Univ. Pittsburgh;
Dmitri Klimov, Professor, Department of Computational Biology, George Mason University;
Ruxandra Dima, Assoc. Prof., Department of Chemistry, Univ. Cincinnati;

Namkung Lee, Professor, Department of Physics, Sejong University, South Korea;
Valeri Barsegov, Assoc. Prof., Department of Chemistry, U. Mass.-Lowell;
Marcos Betancourt, Asst. Prof., Indiana Univ.-Purdue Univ. Indianapolis;
George Stan, Assoc. Prof., Department of Chemistry, Univ. Cincinnati;
Margaret S. Cheung, Assoc. Prof., Department of Physics, Univ. Houston;

S. Vaitheeswaran, Lecturer, University of Massachusetts
Wenjun Zheng, Associate. Prof., Department of Physics, SUNY Buffalo.
Riina Tehver, Associate. Prof., Department of Physics, Denison University;
Sam S. Cho, Associate Prof., Departments of Computer Science and Physics, Wake Forest University;
Zhenxing Liu Associate Prof. Department of Physics, Beijing Normal University (China)

Govardhan Reddy Asst. Prof. Solid State and Structural Chemistry Unit, IISc Bangalore (India)
Jong-Chin Lin (consultant)
Toan M. Ngo (Entrepreneur)
Michael Hincezewski (Asst. Professor, Case Western University, Department of Physics)
Natasha Denesyuk (Consultant)

Pavel Zhuravlev (Banking Consultant)
Upayan Baul (Postdoctoral Fellow, Germany)

Visiting Professors

Late Prof. C. DeDominicis (Saclay, France); Prof. M. S. Li (Polish Academy of Sciences, Warsaw);
Prof. J. Rasaiah (Chemistry, University of Maine); Meng Qin (Nanjing University, China).

PUBLICATIONS

1. "Comparison of Convergence for the Schwinger, Optimized Anomaly-Free and Optimized Minimum-Norm Variational Methods for Potential Scattering", D. Thirumalai and D. G. Truhlar, *Chem. Phys. Lett.* 70, 330-335 (1980).

2. "Excitation of the Asymmetric Stretch of CO_2 by Electron Impact", D. Thirumalai, K. Onda and D. G. Truhlar, *J. Phys. B* 13, L619-L622 (1980).

3. "Elastic Scattering and Rotational Excitation of a Polyatomic Molecule by Electron Impact: Acetylene", D. Thirumalai, K. Onda and D. G. Truhlar, *J. Chem. Phys.* 74, 526-534 (1981).

4. "Electron Scattering by CO_2: Elastic Scattering, Rotational Excitation and Excitation of the Asymmetric Stretch at 10 eV Impact Energy", D. Thirumalai, K. Onda and D. G. Truhlar, *J. Chem. Phys.* 4, 6792-6805 (1981).

5. "Improved Calculation of the Cross Section for Excitation of the Asymmetric Stretch of CO_2 by Electron Impact", D. Thirumalai and D. G. Truhlar, *J. Chem. Phys.* 75, 5207-5209 (1981).

6. "Dispersion-Equation Approach to Obtaining Complex Potentials for Electron Scattering", S. M. Valone, D. Thirumalai and D. G. Truhlar, *Int. J. Quant. Chem. Symp.* 15, 341 (1981).

7. "Full Response Pseudo Channels: A New Method for Converging Coupled-Channel Scattering Calculations: Theory and Examples", D. Thirumalai and D. G. Truhlar, *J. Chem. Phys.* 76, 385-389 (1982).

8. "Polarization and Absorption Effects in e-He Scattering at 30-400 eV", D. Thirumalai, D. G. Truhlar, M. A. Brandt, R. A. Eades and D. A. Dixon, *Phys. Rev. A* 25, 2946-2958 (1982).

9. "A Localized Second-Order Optical Potential for Electron Scattering in Terms of Imaginary Frequency Susceptibilities", S. M. Valone, D. G. Truhlar and D. Thirumalai, *Phys. Rev. A* 25, 3003-3014 (1982).

10. "Application of Variational Matrix Effective Potential Formalism for e-Ne Scattering and Comparisons to Optical Potential Calculations", D. Thirumalai and D. G. Truhlar, *Phys. Rev. A* 25, 3058-3071 (1982).

11. "Rapid Convergence of V-V Energy Transfer Calculations Using Adiabatic Basis Functions. I. An Accurate Two State Model for Low-Energy Resonant V-V Energy Transfer. II.", D. Thirumalai and D. G. Truhlar, *J. Chem. Phys.* 76, 5287-5294 (1982).

12. "Energy Dependent Polarization Potential, Dispersion Relation Absorption Potential and Matrix Effective Potential for Electron-Neon Scattering at 10-100 eV", D. Thirumalai and D. G. Truhlar, *Phys. Rev. A* 26, 793-807 (1982).

13. "Tests of Semiclassical Polarization Approximation for Electron Scattering by Helium and Neon", D. Thirumalai and D. G. Truhlar, *Phys. Rev. A* 27, 158-166 (1982).

14. "Electron Scattering by Methane. Elastic Scattering and Rotational Excitation Cross Sections by ab-Initio Potential", N. Abusalbi, R. A. Eades, T. Nam, D. Thirumalai, D. A. Dixon, D. G. Truhlar and M. Dupuis, *J. Chem. Phys.* 78, 1213-1227 (1983).

15. "Tests of Quasiclassical Trajectory Cross-Correlation Moment Method Against Accurate Quantum Dynamics for V-V Energy Transfer in HF-HF Collisions", D. W. Schwenke, D. Thirumalai, D. G. Truhlar and M. E. Coltrin, *J. Chem. Phys.* 78, 3078-3083 (1983).

16. "Non-Empirical Model for Imaginary Part of the Optical Potential for Electron Scattering", G. Staszewska, D. W. Schwenke, D. Thirumalai and D. G. Truhlar, *J. Phys. B* 16, L281-L287 (1983).

17. "On the Calculation of Time Correlation Functions in Quantum Systems: Path Integral Techniques", D. Thirumalai and B. J. Berne, *J. Chem. Phys.* 79, 5029-5033 (1983).

18. "An Iterative Scheme for the Evaluation of Discretized Path Integrals", D. Thirumalai, E. J. Bruskin and B. J. Berne, *J. Chem. Phys.* 79, 5063-5069 (1983).

19. "Quasifree Scattering Model for the Imaginary Part of the Optical Potential for Electron Scattering", G. Staszewska, D. W. Schwenke, D. Thirumalai and D. G. Truhlar, *Phys. Rev. A* 28, 2740-2751 (1983).

20. "Accurate, Smooth, Local, Energy Dependent Optical Potentials for Electron Scattering", D. W. Schwenke, D. Thirumalai and D. G. Truhlar, *Phys. Rev. A* 28, 3258-3267 (1983).

21. "Rational Fraction Analytic Continuation Method for Complex Resonance Energies in Multidimensional Systems", D. Thirumalai, T. C. Thompson and D. G. Truhlar, *J. Chem. Phys.* 80, 5864-5865 (1984).

22. "Time Correlation Functions in Quantum Systems", D. Thirumalai and B. J. Berne, *J. Chem. Phys.* 81, 2512-2513 (1984).

23. "A Path Integral Monte Carlo Study of Liquid Neon and the Quantum Effective Pair Potential", D. Thirumalai, R. W. Hall and B. J. Berne, *J. Chem. Phys.* 81, 2523-2527 (1984).

24. "Adiabatic and Nonadiabatic Methods for Energies, Lifetimes, and Branching Probabilities of Bimolecular Reactive Collisions", B. C. Garrett, D. W. Schwenke, R. T. Skodje, D. Thirumalai, T. C. Thompson and D. G. Truhlar, A. C. S. Symposia Series 263, 375-400 (1984).

25. "On the Use of Semiclassical Dynamics in Determining Electronic Spectra of Br_2 in Ar Matrix", D. Thirumalai, E. J. Bruskin and B. J. Berne, *J. Chem. Phys.* 83, 230-238 (1985).

26. "Path Integral Methods for Simulating Electronic Spectra", D. Thirumalai and B. J. Berne, *Chem. Phys. Lett.* 116, 471-473 (1985).

27. "Evaluation of Microcanonical Rate Constants for Bimolecular Reactions by Path Integral Techniques", D. Thirumalai, B. C. Garrett and B. J. Berne, *J. Chem. Phys.* 83, 2972-2975 (1985).

28. "Path Integral Monte Carlo Simulations of Electron Localization in Water Clusters", D. Thirumalai, A. Wallqvist and B. J. Berne, *J. Stat. Phys.* 43, 973-984 (1986).

29. "Effect of Elongational Flow on the Isotropic Nematic Phase Transitions in Rod-like Systems", D. Thirumalai, *J. Chem. Phys.* 84, 5869-5873 (1986).

30. "Localization of an Electron in Water Clusters", A. Wallqvist, D. Thirumalai and B. J. Berne, *J. Chem. Phys.* 85, 1583-1591 (1986).

31. "Structure and Dynamics of Screened Coulomb Colloidal Liquids", R. O. Rosenberg and D. Thirumalai, *Phys. Rev. A* 33, 4473-4476 (1986) (Rapid Communication).

32. "Lifshitz Tails in a Spatially Correlated Random Potential", D. Thirumalai, *J. Phys. C* 19, L397-L401 (1986).

33. "On the Simulation of Quantum Systems: Path Integral Methods", B. J. Berne and D. Thirumalai, *Ann. Rev. Phys. Chem.* 37, 401-424 (1986).

34. "On the Use of Dispersion Relations in Obtaining Local Optical Model Potential for Electron Scattering", D. Thirumalai, G. Staszewska, and D. G. Truhlar, *Comm. At. Mol. Phys.* 20, 217-243 (1987).

35. "Flow Induced Transitions in Smectic Liquid Crystals", C. A. Condat and D. Thirumalai, *J. Chem. Phys.* 86, 4548-4554 (1987).

36. "Relaxation of Anisotropic Correlations in (Two Component) Supercooled Liquids", D. Thirumalai and R. D. Mountain, *J. Phys. C* 20, L399-L405 (1987).

37. "Path Integral Monte Carlo Study of the Hydrated Electron", A. Wallqvist, D. Thirumalai and B. J. Berne, *J. Chem. Phys.* 86, 6404-6418 (1987).

38. "Dynamics of the Structural Glass Transition and the p-Spin Interaction Spin Glass Model", T. R. Kirkpatrick and D. Thirumalai, *Phys. Rev. Lett.* 58, 2091-2094 (1987).

39. "Path Integral Monte Carlo Studies of the Behavior of Excess Electrons in Simple Fluids", D. F. Coker, D. Thirumalai and B. J. Berne, *J. Chem. Phys.* 86, 5689-5702 (1987).

40. "Molecular Dynamics Study of Glassy and Supercooled States of a Binary Mixture of Soft Spheres", R. D. Mountain and D. Thirumalai, *Phys. Rev. A* 36, 3300-3311 (1987).

41. "Order-Disorder Transition in Colloidal Suspensions", R. O. Rosenberg and D. Thirumalai, *Phys. Rev. A* 36, 5690-5700 (1987).

42. "p-Spin Interaction Model: Connections with the Structural Glass Problem", T. R. Kirkpatrick and D. Thirumalai, *Phys. Rev B* 36, 5388-5397 (1987).

43. "A Mean Field Soft Spin Potts Glass Model: Statics and Dynamics", T. R. Kirkpatrick and D. Thirumalai, *Phys. Rev. B* 37, 5342-5350 (1988).

44. "Isolated Polymer Molecule in a Random Environment", D. Thirumalai, *Phys. Rev. A* 37, 269-276 (1988).

45. "Freezing of a Colloidal Liquid Subject to Shear Flow", B. Bagchi and D. Thirumalai, *Phys. Rev. A* 37, 2530-2538 (1988).

46. "Electron Localization by Atomic and Molecular Clusters", D. Thirumalai, in Large Finite Systems, 231-240, eds. J. Jortner and B. Pullman (Reidel Publishing, 1988).

47. "A Comparison Between Dynamical Theories and Metastable States in Regular and Glassy Mean Field Spin Models with Underlying First Order Like Transitions", T. R. Kirkpatrick and D. Thirumalai, *Phys. Rev. A* 38, 4439-4448 (1988).

48. "Mean Field Potts Glass Model: Initial Condition Effects on Dynamics and Properties of Metastable States", D. Thirumalai and T. R. Kirkpatrick, *Phys. Rev. B* 38, 4881-4892 (1988).

49. "Random Solutions From a Regular Density Functional Hamiltonian: A Static and Dynamical Theory for the Structural Glass Transition", T. R. Kirkpatrick and D. Thirumalai, *J. Phys. A* 22, L149-L159 (1989).

50. "Polymer Chains in Porous Media", J. D. Honeycutt, D. Thirumalai and D. K. Klimov, *J. Phys. A* 22, L169-L175 (1989).

51. "Ergodic Behavior in Supercooled Liquids and in Glasses", D. Thirumalai, R. D. Mountain and T. R. Kirkpatrick, *Phys. Rev. A* 39, 3563-3574 (1989).

52. "Static Properties of Polymer Chains in Porous Media", J. D. Honeycutt and D. Thirumalai, *J. Chem. Phys.* 90, 4542-4559 (1989).

53. "Liquid and Crystalline States of Monodisperse Charged Colloidal Particles", D. Thirumalai, *J. Phys. Chem.* 93. 5637-5644 (1989).

54. "Scaling and Droplet Notions for the Dynamics of Viscous Liquids Near an Ideal Glassy State", T. R. Kirkpatrick, D. Thirumalai and P. G. Wolynes, *Phys. Rev. A* 40, 1045-1054 (1989).

55. "Liquid, Crystalline and Glassy States of Binary Charged Colloidal Suspensions", R. O. Rosenberg, D. Thirumalai and R. D. Mountain, *J. Phys. Condensed Matter* 1, 2109-2114 (1989).

56. "Probes of Equipartition in Nonlinear Hamiltonian Systems", D. Thirumalai and R. D. Mountain, *J. Stat. Phys.* 57, 789-801 (1989).

57. "Infinite Range Ising Spin Glass in a Transverse Field", D. Thirumalai, Q. Li and T. R. Kirkpatrick, *J. Phys. A* 22, 3339-3349 (1989).

58. "Measures of Effective Ergodic Convergence in Liquids", R. D. Mountain and D. Thirumalai, *J. Phys. Chem.* 93, 6975-6979 (1989).

59. "Dynamical Aspects of Anisotropic Correlations in Supercooled Liquids", R. D. Mountain and D. Thirumalai, *J. Chem. Phys.* 92, 6116-6122 (1990).

60. "Metastability of the Folded States of Globular Proteins", J. D. Honeycutt and D. Thirumalai, *Proc. Natl. Acad. Sci.* 87, 3526-3529 (1990).

61. "Variational Theories for Localized States of an Excess Electron in Fluids", M. R. Shaw and D. Thirumalai, *J. Chem. Phys.* 93, 3460-3470 (1990).

62. "Ergodic Convergences in Liquids and Glasses", R. D. Mountain and D. Thirumalai, *Int. J. Mod. Phys. C* 1, 77-89 (1990).

63. "1/p Expansions for p-Spin Interaction Model in a Transverse Field", V. Dobrosavljevic and D. Thirumalai, *J. Phys. A* 23, L767-L774 (1990).

64. "Ergodic Convergence Properties of Supercooled Liquids and Glasses", D. Thirumalai and R. D. Mountain, *Phys. Rev. A* 42, 4574-4587 (1990).

65. "Influence of Optimal Cavity Shapes on the Size of Polymer Molecules in Random Media", J. D. Honeycutt and D. Thirumalai, *J. Chem. Phys.* 93, 6851-6858 (1990).

66. "Drag Reduction in Turbulent Flows by Polymers", J. K. Bhattacharjee and D. Thirumalai, *Phys. Rev. Lett.* 67, 196-199 (1991).

67. "Ergodic Measures for the Simulation of Dielectric Properties of Water", R. D. Mountain and D. Thirumalai, *Comp. Phys. Comm.* 62, 352-359 (1991).

68. "Methods for Simulating Time Correlation Functions in Quantum Systems", D. Thirumalai and B. J. Berne, *Comp. Phys. Comm.* 63, 415-426 (1991).

69. "Free Polymer in a Colloidal Solution", M. R. Shaw and D. Thirumalai, *Phys. Rev. A* 44, R4797-R4800 (1991).

70. "Topologically Entangled Polymers", D. Thirumalai, *Theor. Chem. Acta.* 82, 407-417 (1992).

71. "The Nature of Folded States of Globular Proteins", J. D. Honeycutt and D. Thirumalai, *Biopolymers* 32, 695-709 (1992).

72. "Ergodicity and Activated Dynamics in Supercooled Liquids", R. D. Mountain and D. Thirumalai, *Phys. Rev. A* 45, R3380-R3383 (1992).

73. "Loss in Ergodicity in Supercooled Liquids", R. D. Mountain and D. Thirumalai, "Slow Dynamics in Condensed Matter", edited by K. Kawazaki, T. Kawakatsu, and M. Tokuyama, AIP Conference Proceedings, 256, 165-172 (1992).

74. "Folding Kinetics of Proteins: A Model Study", Z. Guo, D. Thirumalai and J. D. Honeycutt, *J. Chem. Phys.* 97, 525-535 (1992).

75. "Conformations of Polyelectrolyte Chain", B.-Y. Ha and D. Thirumalai, *Phys. Rev. A* 46, R3012-R3015 (1992).

76. "Theoretical Probes of Conformational Fluctuations in Proteins with Applications to S. Peptide and RNase A/3' - UMP Enzyme/Product Complex", J. E. Straub and D. Thirumalai, *Proteins: Structure, Function, and Genetics* 15, 360-373 (1993).

77. "Kinetics and Thermodynamics of Folding in Model Proteins", C. J. Camacho and D. Thirumalai, *Proc. Natl. Acad. Sci.* 90, 6369-6372 (1993).

78. "Exploring the Energy Landscape in Proteins", J. E. Straub and D. Thirumalai, *Proc. Natl. Acad. Sci.* (USA) 90, 809-813 (1993).

79. "Relationship Between the Fluctuation Metric and the Non-ergodicity Parameter: Incoherent Scattering Function", R. D. Mountain and D. Thirumalai, *Physica A* 192, 543-549 (1993).

80. "Activated Dynamics, Loss of Ergodicity, and Transport in Supercooled Liquids", D. Thirumalai and R. D. Mountain, *Phys. Rev. E* 47, 479-489 (1993).

81. "Minimum Energy Compact Structures of Random Sequences of Heteropolymers", C. J. Camacho and D. Thirumalai, *Phys. Rev. Lett.* 71, 2505-2508 (1993).

82. "Dynamics in Rugged Energy Landscapes with Applications to the S-peptide and Ribonuclease A", J. E. Straub, A. B. Rashkin, and D. Thirumalai, *J. Amer. Chem. Soc.* 116, 2049-2063 (1994).

83. "Rotational Relaxation of a Spherocylinder and a Semirigid Molecule in Concentrated Solutions", D. Thirumalai, *J. Phys. Chem.* 98, 9265-9269 (1994).

84. "Theoretical Perspectives on *in vitro* and *in vivo* Protein Folding", D. Thirumalai, in *Statistical Mechanics, Protein Structure, and Protein Substrate Interactions*, edited by S. Doniach p. 115-134, (Plenum Press, NY, 1994).

85. "Quantitative Measure of Efficiency of Monte Carlo Simulations", R. D. Mountain and D. Thirumalai, *Physica A* 210, 453-460 (1994).

86. "Theoretical Predictions of Folding Pathways Using the Proximity Rule with Applications to BPTI", C. J. Camacho and D. Thirumalai, *Proc. Natl. Acad. Sci.* 92, 1277 (1995).

87. "Nucleation Mechanism for Protein Folding and Theoretical Predictions for Hydrogen-Exchange Labelling Experiments", D. Thirumalai and Z. Guo, *Biopolymers* (Research Communications 37, 137-140 (1995)).

88. "Modeling Disulfide Bonds in Globular Proteins: Entropic Barriers and Pathways", C. J. Camacho and D. Thirumalai, *Proteins: Structure, Function and Genetics*, 22. 28-40 (1995).

89. "Kinetics of Protein Folding: Nucleation Mechanism, Time Scales, and Pathways", Z. Guo and D. Thirumalai, *Biopolymers*, 36, 83-102 (1995).

90. "Electrostatic Persistence Length of a Polyelectrolyte Chain", B. Ha and D. Thirumalai, *Macromolecules* 28, 577-581 (1995).

91. "The Cavity Approach to Metastable Glassy States Near Random First Order Phase Transition", T. R. Kirkpatrick and D. Thirumalai, *J. Physique I* 5, 771-786 (1995).

92. "Are Disordered Spin Models Relevant for the Structural Glass Problem?", T. R. Kirkpatrick and D. Thirumalai, *Transp. Theory and Stat. Mech.,* 24, 927-945 (1995).

93. "From Minimal Models to Proteins: Time Scales for Protein Folding Kinetics", D. Thirumalai, *J. Physique* (Paris), 5, 1457-1467 (1995).

94. "Navigating the Folding Routes", P. G. Wolynes, J. Onuchic, and D. Thirumalai, *Science*, 267, 1619-1620 (1995).

95. "A Mean Field Model for Semiflexible Chains", B. Y. Ha and D. Thirumalai, *J. Chem. Phys.*, 103, 9408-9412 (1995).

96. "Energy Landscape and Folding Mechanisms in Proteins", Z. Guo and D. Thirumalai, *In Protein Folds: a distance based approach* edited by H. Bohr and S. Brunak (CRC Press, Boca Raton, FL, 1995) 233-239.

97. "Analytical Theories of Protein Folding", T. Garel, H. Orland, and D. Thirumalai, in *New Developments in Theoretical Studies of Protein Folding* edited by R. Elber (World Scientific, 1996) pp. 197-268.

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356. "Chromatin is stretched but intact when the nucleus is squeezed through constrictions", D. Thirumalai and G. Shi, *Biophys. J.* **112:** 411-412 (2017).
357. "Collapse precedes folding in denaturant assembly of Ubiquitin", G. Reddy and D. Thirumalai, *J. phys. Chem. B.* **121:** 995-1009 (2017).
358. "Protein collapse is encoded in Native State Architecture", H. S. Samanta, P. Zhuravlev, M. Hinczewski, N. Hori, S. Chakrabarty, and D.Thirumalai, *Soft Matter*, **13:** 3622-3638 (2017).
359. "Ripping RNA by force Using Gaussian Network Models", C. Hyeon and D. Thirumalai, *J. Phys. Chem.* **121:** 3515-3522 (2017).
360. "Kinematics of Lever Arm Swing in Myosin VI", M. L. Mugnai and D. Thirumalai, *Proc. Natl. Acad. Sci.,* **114:** E4389-E4398 (2017).
361. "Thermodynamics of Helix-Coil transitions of polyalanine in open carbon nanotubes", D. Suvlu, S. Senavirtane, D. Thirumalai, and J. Rasaiah, *J. Phys. Chem. Lett.*, **8:** 494-499 (2017).
362. "Optimal information transfer in enzymatic networks: A field theoretic formulation", H. S. Samanta, M. Hinczewski, and D.Thirumalai, *Phys. Rev.E.* **96:** 012406 (2017).
363. "Ultrasensitivity of Water Exchange Kinetics to the size of the metal cation", Y. Lee, D. Thirumalai, and C. Hyeon, *J. Am. Chem. Soc.* **139:** 12324-12327 (2017).
364. "Parsing the roles of neck-linker docking and tethered head diffusion in the stepping dynamics of kinesin", Z. Zhang, Y. Goldtzvik, and D. Thirumalai, *Proc. Natl. Acad. Sci.***114:** (46) E9838-E9845 (2017).
365. "Molecular chaperones maximize the native state yield on biological times by driving substrates out of equilibrium", S. Chakrabarti, C. Hyeon, X. Ye, G. H. Lorimer, and D. Thirumalai, *Proc. Natl. Acad. Sci.* **114:** E10919 – E10927 (2017).

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366. "Denaturants alter the flux through multiple pathways in the folding pathways of PDZ domain", Z. Liu and D. Thirumalai, *J. Phys. Chem. B.***122:** 1408-1416 (2018).
367. "Forced-adhesion of Cell Adhesion complexes reveals abrupt switch between two brittle states", *J.Chem. Phys.* N. M. Toan and D. Thirumalai, **148:** 123332 (2018).
368. "Cell growth dictates the onset of glass to fluid-like transition and long time super diffusion in an evolving cell colony", A. M. Kakkada, X. Li, H. S. Samanta, S. Sinha, and D. Thirumalai, *Phys. Rev. X.* **8:** 021025 (2018).
369. "Signaling networks and dynamics of allosteric transitions in bacterial chaperonin GroEL: Implications for Iterative Annealing of misfolded proteins", D. Thirumalai and C. Hyeon, *Phil. Trans. Royal Soc. B* **373:** 20170182 (2018).
370. "Structure of APP C-99 1-99 and implications for extra-membrane domains in function and oligomerization" *Biochemica et Biophysica Acta-Biomembranes,* G. A. Pentalapulos, J.E. Straub, D. Thirumalai, and Y. Sugita **1860: (9)**, 1698 – 1708 (2018).
371. "Sequence-dependent Three Interaction Site Model for Single- and Double-stranded DNA", D. Chakraborty, N. Hori, and D. Thirumalai, *J. Chem. Theor. & Comp.,* **14:** 3763-3779 (2018).
372. "Interphase Chromosome Exhibits Out of Equilibrium Glassy Dynamics", G. Shi, L. Liu, C. Hyeon, and D. Thirumalai, *Nat. Comm.* **9:** 3161 (2018) DOI: 10.1038/s41467-018-05606-6.

Highlighted in https://twitter.com/NSF_MPS/status/1040685172470042624

373. "Charge fluctuation effects on he shape of flexible polyampholytes with applications to intrinsically disoodered protein", H. S. Samanta, D. Chakraborty, and D. Thirumalai, *J. Chem. Phys*. **149 (6):** 163323 (2018).
374. "Interface residues that drive allosteric transitions also control the Assembly of L-lactate dehydrogense", J. Chen and D. Thirumalai, *J. Phys. Chem. B* **122:** 11195-11205 (2018).
375. "Frictional effects on RNA Folding: Speed Limit and Kramers turnover", N. Hori, N. A. , Denesyuk, and D. Thirumalai, *J. Phys. Chem. B* **122:** 11279-11288 (2018).
376. "Monovalent ions modulate the flux through multiple folding pathways of an RNA pseudoknot", J. Roca, N. Hori, S. Baral, Y. Velmurugu, R. Narayanan, P. Narayanan, D. Thirumalai, and A. Ansari, *Proc. Natl. Acad. Sci*. **115: (31),** E7313-7322 (2018).
377. "Forced-rupture of cell-adhesion complexes reveals abrupt switch between two brittle states", N. M Toan and D. Thirumalai, *J. Chem. Phys*. **148:** (12), 123332 (2018).
378. "Regulatory element in fibrin triggers tension-activated transition from catch to slip bonds", R. I. Litvinov, O. Kononova, A. Zhmurov, K. A. Marx, V. Barsegov, D. Thirumalai, and J. W. Weisel, *Proc. Natl. Acad. Sci.* **115:** (34), 8475 – 8480 (2018).
379. "Synergy between intrinsically disordered domains and structured proteins amplifies membrane curvature sensing", W. Zeno, U. Baul, W. Snead, A.C.M. De Groot, L. Wang, E. M. Lafer, D. Thirumalai, and J. Stachowiak, *Nat. Communications* **9:** 4152 (2018).
380. "Interface residues that drive Allosteric Transitions Also Drive Assembly of L-Lactate Dehydrogenase" J. Chen and D. Thirumalai, *J. Phys. Chem. B*. **122:** 11195 – 11205 (2018).
381. "Dynamics of Allosteric Transitions in Dynein", Y. Goldtzvik, M. Mugnai, and D. Thirumalai, *Structure*, **26:** 1664 (2018). **Cover Illustration**
382. "Molecular Simulations of ion Effects on the Thermodynamics of RNA Folding", N.A. Denesyuk, H, Hori, and D. Thirumalai, *J. Phys. Chem. B.*, **122:** 11860-11867 (2018).

2019.

383. "Share, but unequally: A plausible Mechanism for the Emergence and Maintenance of Intratumor Heterogeneity", *J. Roy. Soc. Int.*, **16:** 20180820 (2019).
384. "Origin of Super Diffusive Behavior in a Class of Non-Equilibrium Systems", H. S. Samanta and D. Thirumalai, *Phys. Rev. E.*, **99:** 032401 (2019).
385. "Sequence Effects on size, shape, and structural heterogeneity in Intrinsically Disordered Proteins", U. Baul, D. Chakraborty, M. L. Mugnai, J. E. Straub, and D. Thirumalai, *J. Phys. Chem. B.* **123:** 3462-3474 (2019).
386. "Ion Condensation onto Ribozyme is Site Specific and fold dependent", N. Hori, N.A. Denesyuk, D. Thirumalai, *Biophys. J.* **116:** 2400-2410 (2019). Commentary: *Biophys. J.* **116:** 2237-2239.
387. "Processivity, Velocity, and Universal Characteristics of Nucleic Acid Unwinding by Helicases", S. Chakraborty, C. Jarzynski, and D. Thirumalai, *Biophys. J.* **117:** 867-879 (2019).
388. "Symmetry, Rigidity, and Allosteric Signaling: From Monomeric Proteins to Molecular Machines", D. Thirumalai, Changbong Hyeon, P. I. Zhuravlev, and G. H. Lorimer, *Chemical Reviews* **119:** 6788 – 6821 (2019); **Cover Illustration.**

389. "Universal Nature of Collapsibility in the context of protein folding and Evolution", D. Thirumalai, H. S. Samanta, H. Maity, and G. Reddy, *Trends in Biochem. Sci.* **44:** 675-687 (2019).
390. "Sequence Effects on Size, Shape, and Structural Heterogeneity in Intrinsically Disordered Proteins", U. Baul, D. Chakraborty, M. L. Mugnai, J. E. Straub, and D. Thirumalai, *J. Phys. Chem. B.***123:** 3462-3474 (2019).
391. "Theory and simulations for RNA folding in a mixtures of monovalent and divalent cations", H. T. Ngyuen, N. Hori, and D. Thirumalai, *Proc. Natl. Acad. Sci.* **116:** xxxx-xxx (2019).
392. "How kinesin waits for ATP affects the nucleotide and load dependence of the stepping kinetics", R. Takaki, M. L. Mugnai, Y. Goldtzvik, and D. Thirumalai, **116:** xxx-xxx (2019).
393. "Conformational Heterogeneity in human interphase chromosome organization reconciles the FISH-Hi-C paradox", *Nat. Comm.* **10:** 3894 (2019).

INVITED TALKS (Since 1994)

1. Department of Physics, University of Pittsburgh May 12, 1994.
2. ACS Meeting, Washington, D.C., "Flow Induced Structure in Polymers", August 22, 1994.
3. Workshop on "Biomolecular Materials", Institute of Theoretical Physics, Santa Barbara, August 26, 1994.
4. National Institutes of Health, Bethesda, MD, November 4, 1994.
5. Symposium on Distance-Based Approach to Protein Structure Determination II (Copenhagen, Denmark) November 11, 1994.

6. Los Alamos National Labs, New Mexico, January 18, 1995.
7. APS Meeting, March, 1995 (invited talk).
8. University of Pennsylvania, Department of Chemistry, March 30, 1995.
9. Department of Physics, University of California at San Diego, April 27, 1995.
10. International Meeting in Disordered Systems and Spin Glasses, Saclay, France, July, 1995.

11. "Physics of Biology: from Molecules to Species", Humlabek, Denmark, August, 1995.
12. Department of Chemistry, Brown University, December 1995.
13. Physics and Biology: Aspen Winter Meeting, January 1996.
14. National Institutes of Health, Bethesda, MD, February 2, 1996.
15. Department of Physics, Pennsylvania State University, University Park, PA, February 9, 1996.

16. Department of Physical Chemistry, Hebrew University, Jerusalem, April 15, 1996.
17. Department of Physics, University of California, Santa Barbara, CA, May, 1996.
18. Department of Chemistry, University of California, Los Angeles, CA, May, 1996.
19. Indian Institute of Cultivation Sciences, Calcutta, India, July, 1996.
20. International Center for Theoretical Physics, Trieste, Italy, July, 1996 (2 hours).

21. International Center for Theoretical Physics, Trieste, Italy, August 1, 1996 (2 hours).
22. International Center for Theoretical Physics, Trieste, Italy, August 2, 1996 (2 hours).
23. American Chemical Society Meeting, Protein Folding, Orlando, FL, May, 1996.
24. Institute for Physical Science and Technology, University of Maryland, College Park, MD, September, 1996.
25. Cornell Theory Center, Cornell University, Ithaca, NY, October, 1996. (45 minutes).

26. Supercomputer Center, University of Minnesota, Minneapolis, MN, December, 1996).
27. Statistical Mechanics Meeting, Rutgers, NJ, December, 1996. (25 minutes).
28. Rockefeller University, Center for Physics and Biology, New York, May 1997.
29. Conference in Julich, Germany on Monte Carlo Methods in Protein Folding, December 1997.
30. Department of Biochemistry, University of Regansburg, December 1997.
31. Biozentrum, Basel, Switzerland, December 1997.
32. American Physical Society Meeting, March 1998, Los Angeles, (45 min.)
33. CECAM Workshop on Protein Structure and Function, June, 1998, Torino, Italy.
34. Conference on “Computations in Protein Folding”, Institute for Advanced Study, Hebrew University, Jerusalem, October, 1998.

35. Special Lecture on "Protein Folding Kinetics I", Institute for Advanced Study, Hebrew University, Jerusalem, November, 1998, (90 min.)

36. Special Lecture on "Protein Folding Kinetics II", Institute for Advanced Study, Hebrew University, Jerusalem, November, 1998, (90 min.)
37. Colloquium Weizmann Institute, Rehovot, Israel, December, 1998.
38. Colloquium Tel Aviv University, Rehovot, Israel, December, 1998.
39. University of Regensburg, Germany, "Regensburger Faltertag" (protein folding meeting) April, 1999.
40. Department of Chemistry, Louisiana State University, April, 1999.

41. Department of Physics, Michigan Technological University, May, 1999.
42. CECAM Meeting on "Phase Space and Energy Landscape in Disordered Systems", Lyon, France (Plenary Lecture), June, 1999.
43. 4th Claude Itzykan Meeting on "Soft Condensed Matter Physics", Saclay, France, June, 1999.
44. Conference on "Stochastic Dynamics and Pattern Formation in Biological Systems" (Seoul, Korea) July, 1999.
45. Conference on "Complex Material Science", University of California, Santa Barbara, August, 1999.

46. CECAM Workshop "Algorithm for Enhanced Sampling in Simulations of Condensed Matter Systems", Lyon, France, September, 1999.
47. Protein Folding Symposium in honor of G. Nemethy, Mount Sinai Medical Scool, New York, October, 1999.
48. Biophysics Colloquium, Cornell University, October, 1999.
49. Department of Chemistry, SUNY, Stonybrook, November, 1999.
50. Department of Biophysics, Johns Hopkins University, November, 1999.

51. Scripps Research Institute, February 4, 2000.
52. IBM Research Laboratory, February 16, 2000.
53. 41st Quantum Chemistry Sanibel Symposium, March 3, 2000.
54. International Conference on Protein Folding, Torino, Italy, April, 2000.
55. National Cancer Institute, Frederick, MD, July 2000.

56. Nineteenth Annual Symposium on Molecular Biology, "Proteins and RNA Folding: Sharing Perspectives", Penn-State University, August 3, 2000
57. Quantum Biology Symposium, New Orleans, August 15, 2000.
58. Nagoya Conference on "Proteins in Protein Folding", Okazaki, Japan, October 16-18, 2000.
59. University of Nagoya, October 19, 2000.
60. Department of Physics, University of Illinois, December 4, 2000.

61. Danforth Center and Washington University, St. Louis, February 8, 2001.
62. Institute for Theoretical Physics, UCSB, February 23, 2001.
63. National Institutes of Health, March 13, 2001.
64. National American Chemical Society Meeting, San Diego, April 4, 2001 (40 minutes).
65. National Institutes of Health, May 10, 2001.

66. Conference on "Electrostatic Interactions in Polymers, Colloids, and Biophysics", Minneapolis, MN, May 12, 2001 (40 minutes).
67. Institute for Physical Science and Technology, University of Maryland, May 15, 2001.
68. IBM Yorktown Heights, May 22, 2001.
69. Institute for Mathematical Sciences, Chennai, India, August 2, 2001.
70. Department of Chemistry, Columbia University, New York, September 6, 2001.

71. Symposium on "The Role of Protein Structure Prediction in the Post-Enomic Era" (celebrating the 80th Birthday of Prof. H. A. Scheraga), Cornell University, Ithaca, NY, October 25, 2001.
72. Department of Bioinformatics, George Mason University, VA, October 30, 2001.
73. Laboratoire d'Enzymologie et Biochemie Structurales, Gif-sur-Yvette, France, November 26, 2001.
74. "Folding and self-assembly of Macromolecules," Institut Des Hautes Etudes Scientifiques, Bures-sur-Yvette, France (2 hr. lecture), November 28, 2001.
75. Cambridge Health Institute Meeting on "Protein Expression", San Diego, CA, January 7, 2002.

76. U.S.-Japan NSF meeting on Protein Folding, January 12, 2002.
77. Winter Gordon Research Conference, "Protein Folding and Dynamics," January 24, 2002.
78. Department of Chemistry, University of Pittsburgh, February 5, 2002.
79. Department of Chemistry, University of Wisconsin, February 12, 2002.
80. Department of Physics, Wake Forest University, April, 2002.

81. American Chemical Society Meeting, August, 2002.
82. Computational Biology and Bioinformatics Center, University of Pittsburgh, May, 2002.
83. Single Molecule Conference, Germany, June, 2002.
84. Department of Molecular Genetics, University of Pittsburgh, July, 2002.
85. Department of Physics, Iowa State University, September 18, 2002.

86. Department of Chemistry, University of Pennsylvania, October 10, 2002.
87. International Conference on Dynamics of Complex Systems, University of Florence, Italy.
88. International Conference on Protein Dynamics, Okazaki, Japan, March, 2003.
89. Department of Chemistry, Emory University, Georgia, April 2003.
90. Department of Pharmaceutical Chemistry, University of California, San Francisco, May, 1, 2003.

91. Workshop on Protein Folding, International Center for Theoretical Physics, Trieste, May 12, 2003.
92. Workshop on Protein Folding, ICTP, Trieste (second lecture), May, 14, 2003.
93. Workshop on Protein Folding, Cambridge University, UK, March 2004.
94. Conference on Protein Aggregation, Santa Fe Institute, April 2004.
95. International Conference on Nonlinear Dynamics, Chennai, India, July 2004.

96. Conference on Biological Systems, Rice University, December 2004.
97. NSF Workshop on Biophysics, Arizona State University, May 2004.
98. ACS Meeting, Anaheim, California, March 2004.
99. Department of Chemistry, Rice University, March 8, 2004.
100. Department of Chemistry, University of California, Los Angeles, March 2006.

101. International Optical Spectroscopy of Biomolecular Dynamics, Eilat, Israel, March 22, 2006.

102. ICTP Trieste Conference, Trieste, Italy, July 29, 2006.
103. Department of Chemistry, Massachusetts Institute of Technology, May 8, 2006.
104. Lyon Single Molecule Meeting, Lyon, France, September 30, 2006.
105. Department of Chemistry, University of Texas, Austin, Texas, October 25, 2006.

106. Southwest Theoretical Chemistry Conference, Austin, Texas, October 27, 2006.
107. Carolina Biophysics Symposium, Chapel Hill, North Carolina, November 1, 2006.
108. COE21 International Conference, Perspectives in Nonlinear Physics, University of Tokyo, Tokyo, Japan, November 22, 2006.
109. International Conference on "Nucleation, Aggregation, and Growth" (Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore, India) January 31, 2007.
110. Center for Computational Biology, University of Washington, St. Louis, Feb. 16, 2007.

111. Protein Folding Conference, APS meeting, Denver, CO, March 5, 2007.
112. ACS Meeting on Biophysics of RNA, March 25, 2007.
113. "From computational Biophysics to System Biology", Forschungzentrum, Julich, May 4, 2007.
114. "RNA in Biology, Bioengineering and Nanotechnology," Institute for Mathematics and its Applications, University of Minnesota, Minneapolis, November 1, 2007.
115. "Protein Folding and Dynamics", Key Note Speaker, Gordon Conference, Ventura, CA , January 2008.

116. ACS Meeting, March 2008.
117. Cornell University, May 1, 1008.
118. University of Chicago, May 16, 2008.
119. Single Molecule Symposium in honor of Prof. W.E. Moerner (Wolf Prize, 2008) Tel Aviv University, May 25, 2008.
120. Bar-Ilan University, May 29, 2008.

121. Weizmann Institute, June 1, 2008.
122. " From Macomolecular to Cell Biophysics," – A symposium in honor of Avinoam Ben-Shaul, Hebrew University, June 3, 2008.
123. "Loop formation kinetics in polymers and peptides", in "New challenges in Protein Science" – A symposium in honor of William A. Eaton, Parma, June 5, 2008.
124. Protein Folding Meeting, Rome, June 10, 2008.
125. Protein Society Meeting, July 29, 2008.

126. ACS Meeting on Protein Folding, August 17, 2008.
127. International Workshop on "Current Problems in Soft Condensed Matter," KAIST, Korea September 9, 2008.
128. International conference 2008 "Computational Protein Structure Mechanics", Partner Institute for Computational Biology, Shangai, China, September 12, 2008.
129. "Complex Nanosystems: Assembly, Control and Functionality", San Servolo, Italy. October 2, 2008.
130. XI Annual Single Molecule Linz Winter Workshop, Linz, Austria, February 8, 2009.

131. APS Meeting on Constrained Polymers, Pittsburgh, March 19, 2009 (36 minutes).
132. Biophysics Colloquium, University of Michigan, March 20, 2009.
133. "Enzyme fluctuations during a reaction cycle," Symposium on "*Functional Motions in Enzyme Catalysis,*" ACS Meeting, Salt Lake City, March 23, 2009.
134. "Molecular transfer model for osmolyte effects on protein folding," Symposium on *"The Influence of Ions and Osmolytes on Aqueous Macromolecules",* ACS Meeting, Salt Lake City, March 23, 2009.
135. "Protein Misfolding: Chaperones to the rescue", Biophysics Colloquium, Florida State University, Tallahassee, April 7, 2009.

136. "Growth mechanism of amyloid fibrils," The American Society for Biochemistry and Molecular Biology meeting on "*Protein Folding, Aggregation and Chaperones Meeting*", New Orleans, April 21, 2009.
137. Key Note Speaker "Frontiers in Bio-molecular Aggregation: Experiments, Applications and Simulations", Cecam Workshop, Dublin, Ireland, April 30, 2009.
138. "Folding landscape of RNA from single molecule trajectories", Institute for Mathematical Analysis, *Molecular Simulations: Algorithms, Analysis, and Applications*, May 20, 2009.
139. "Folding Landscape of RNA Hairpins from Single Molecule Force Spectroscopy"*, Mainz Material Simulation Days,* in Max-Planck Institut fur Polymerforsching, Mainz, June 4, 2009.
140. "Structural Basis of Allosteric Transitions in Biological Machines: Common Themes," Keystone Symposia *"Protein Dynamics, Allostery and Function*", June 7, 2009.

141. "Growth mechanism of oligomers and fibrils of amyloidogenic peptides", *Proteins Gordon Research Conference*, Holderness, New Hampshire, June 23, 2009.
142. "*International Meeting on Protein Dynamics,"* Beijing, August 2009
143. "Growth mechanisms in oligomers and fibrils of amyloidogenic peptides", ACS National Meeting, Washington, DC, August 17, 2009.
144. "Chaperonin-Mediated Protein Folding", Seminar, Pennsylvania State University, Biological Chemistry Series, September 15, 2009.
145. "Universality and Specificity in Protein Folding", *Computational Biology of the Cell: The Next Decade",* University of Illinois at Urbana-Champaign, September 22, 2009.

146. "Folding Landscapes of RNA from Single Molecule Force Spectroscopy", Department of Physics, University of Pennsylvania, September 30, 2009.
147. "Chaperonin-assisted folding of Proteins", Department of Chemistry, University of Pennsylvania, October 1, 2009.
148. "Folding landscape of RNA using Single Molecule Force Spectroscopy", Chung-Ang University, Korea, International Meeting Single Molecules, October 7, 2009.
149. "Growth Dynamics of Oligomers and Amyloid Fibrils", 9th KIAS-SNU conference on "Protein Structure and Function," October 8, 2009.
150. "Growth Dynamics of Oligomers and Amyloid Fibrils", Institute of Computational Engineering and Sciences, University of Texas, Austin, November 4, 2009.

151. "Allosteric Transitions and Function in a Biological Nanomachine" "Frontiers in Biomolecular Simulations" International Meeting, Georgia Tech University, November 17, 2009.
152. Colloquium, "Chaperonin-Mediated Protein Folding" Department of Physics, Technical University Munich, December 12, 2009.
153. "Folding of RNA hairpins, riboswitches and ribozymes", Department of Chemistry, Rice University "January 6, 2010
154. "Perspectives on Protein folding", Graduate Research Seminar (Gordon Research Conference meeting on Protein Folding), Ventura CA , January 9, 2010.
155. University of North Carolina Medical School, Department of Biophysics, March 3, 2010.

156. "Allosteric transitions in Biological machines" American Chemical Society Meeting, March 25, 2010,
157. "Keystone Symposium on Computer-Aided Drug Discovery," Whistler, Canada, April 23, 2010.
158. "Folding landscape of RNA from Single Molecule Force Spectroscopy" Joint BU/Harvard/MIT Seminar [2 hours], May 5, 2010.
159. "Physics Colloquium Science at the Edge Series," Michigan State University, May 7, 2010.
160. "Protein Folding Pathways," Arizona State University, May 12, 2010.

161. "Finite-Size effects in Protein Folding", Technical University Munich, Department of Physics, June 24, 2010.
110. (Key Note Speaker) 3DSig "Allostery in Biological Machines" July 10, 2010
163. Conference on Nucleation, Aggregation, and Growth, JNCASR, Bangalore, India "Protein Aggregation: From Oligomers to Fibrils" July 30, 2010
164. Summer School JNCASR, Bangalore "Topics in Protein Folding" (90 minutes) Lecture I, August 2, 2010.
165. Summer School JNCASR, Bangalore, "Single Molecule Force Spectroscopy: Theory and Applications" (90 minutes) Lecture II, August 2, 2010.

166. ACS meeting Boston University, August 25, 2010.
167. Colloquium Department of Chemistry Duke University"Chaperonin-mediated Protein folding", September 28, 2010.
168. Colloquium Department of Chemistry University of Delaware "Protein Folding: Chaperonin to the rescue", October 1, 2010.
169. Workshop on Protein Folding, Lausanne Switzerland, "Chaperonin-mediated protein folding: Realities and Models", October 7, 2010.
170. BioPhysics colloquium "Chaperonin-Mediated Protein folding", RPI, November 12, 2010.

171. 104th Statistical Mechanics Rutgers University "Essence of Tethered Diffusion of Myosin V under load" December 19, 2010.
172. "Chaperones as Biological Nanomachines", Biophysics Colloquium Los Alamos National Laboratory, NM, March 1, 2011.

173. "Confinement & Crowding Effects on Folding Entropy-driven transitions", Biophysical Society Meeting, Baltimore, March 5, 2011.

174. "Chaperonin-mediated protein Folding", Colloquium Arizona State University, March 30, 2011.

175. "Chaperones as Molecular Machines", Department of Physics, SUNY Buffalo, April 6, 2011.

176. "Chaperonin-mediated Protein Folding", CBMG Seminar Series, University of Maryland, College Park, April 7, 2011.

177. "Link between folding landscapes and gene expression of riboswitches", D. E. Shaw Research, New York, NY, April 22, 2011.

178 "Chaperones as Molecular Machines", UMBC, Baltimore, May 3, 2011.

179. Distinguished Scientific Leader Lecture, "Link between folding landscapes and gene expression of riboswitches" Georgia Tech, GA, May 11, 2011.

180. "Architectural basis of functions of biological Machines", Black Forest Focus on Soft Matter 5: Self-Assembly on All Scales, May 27, 2011.
181. "Link between folding landscapes and gene expression of riboswitches" Zurich, May 30, 2011.
182. "Collapse Kinetics and Chevron plots", 17th Albany conversation, Buffao, NY, June 14, 2011.

183. "Crowding effects on protein folding and aggregation", International Congress in Biological Physics, San Diego, CA, June 25, 2011.

184. ACTC "Architectural basis of functions of biological Machines", Telluride, CO, July 18, 2011.

185. "Link between folding landscapes and gene expression of riboswitches", International Conference on Sub cellular dynamics, KIAS, Seoul, Korea, July 25 2011.

186. "Pictures, Models, and reality in protein folding", Molecular Kinetics Conference, Berlin, Germany, September 6, 2011.

187. "Crowding and confinement effects on protein and RNA folding", Scheraga 90th Birthday Symposium, Cornell University, Ithaca, September 24, 2011.
188. "A Primer on Single Molecule Force Spectroscopy", Lecture-I (3 hours) EPFL Lausanne , Switzerland, October 6, 2011.

189. "A Primer on Single Molecule Force Spectroscopy", Lecture-II (3 hours) EPFL Lausanne , Switzerland, October 13, 2011.
190. "A Primer on Single Molecule Force Spectroscopy", Lecture-III (3 hours) EPFL Lausanne , Switzerland, October 20, 2011.

191. "Motility of Molecular Motors", Department of Physics, Nanjing University, December 12, 2011.

2012

192. "Gene regulation by Riboswitches: From folding landscapes to System Level Description", Department of Chemistry, UC San Diego, January 23, 2012.
193. "Gene regulation by Riboswitches: From folding landscapes to System Level Description",

Department of Chemistry, University of Illinois Urbana, February 6, 2012.

194. "Gene regulation by Riboswitches: From folding landscapes to System Level Description", Department of Physics, Georgia Tech University, February 15, 2012.
195. "Role of water in protein aggregation and amyloid polymorphism", APS meeting, Boston, February 2012.
196. "Gene regulation by Riboswitches: From folding landscapes to System Level Description", International meeting on, "Forces in Biomolecular systems", Venice, Italy, March 26, 2012
197. "Gene regulation by Riboswitches: From folding landscapes to System Level Description", Chemistry Colloquium, Carnegie Mellon University, April 12, 2012.
198. "Gene regulation by Riboswitches: From folding landscapes to System Level Description", Chemical Engineering Colloquium, Washington University, St. Louis, April 21, 2012.
199. "Gene regulation by Riboswitches: From folding landscapes to System Level Description", Department of Physics, University of Houston, April 24 2012.
200. "Control of Gene expression by Riboswitches", NIDDK, National Institutes of Health, Bethesda, May 10, 2012.

201. "Role of water in protein aggregation and amyloid polymorphism", GRC Conference on Bioplymers, June 4, 2012.
202. "Crowding and confinement effects on proteins and RNA", International Conference on Molecular Crowding, Monte Verita, Locarno, Switzerland, June 12, 2012 (Keynote Speaker).
203. "Allosteric transitions in Molecular Machines", International workshop on "The emerging dynamic view of proteins: Protein Plasticity in Allostery, Evolution, and Self-assembly" Max Plank Institue for Complex Systems, Dresden, Germany, July 18, 2012.
204. "From folding trajectories to Free energy landscapes", International meeting on "Single Molecule Kinetics", Physikencentrum Bad Honnef (Germany), July 31, 2012.
205. "Function of GroEL follows the Iterative Annealing Mechanism", International Symposium on "Protein Folding and Dynamics", National Center for Biological Sciences, Bangalore, India, October 17, 2012.

2013

206. "Structures of Amyloid Precursor Protein in a Membrane Environment", 2nd International Symposium on Higher Order Structure of Protein Therapeutics", February 11, 2013, Baltimore, MD.
207. "Gene regulation by Riboswitches: From folding landscape to system level description", ACS meeting New Orleans, April 7, 2013.
208. "Structures of Amyloid precursor protein a membrane environment", ACS meeting New Orleans, April 8, 2013.
209. "Crowding Effects on RNA and Protein folding", Computational Biology: Then and now, Weizmann Institute of Science, Rehovat, Israel, May 7, 2013.
210. "Gene regulation by Riboswitches: From folding landscape to system level description", Colloquium Department of Physical Chemistry, Hebrew University, Jerusalem, May 9, 2013.

211. "Protein Folding: From Theory to Practice" Colloquium Montpellier, France May 21, 2013.
212. "Orland and Biophysics" Celebration in honor of H. Orland, CEA Saclay, May 23, 2013.
213. "International conference in Subcellular Dynamics", KIAS, Seoul June 12, 2013.

214. "Molecular Mechanisms and Physiological Consequences of Protein Aggregation" FASEB meeting Big Sky Montana, June 25, 2013 "Structure of Amyloid Precursor Protein in Membranes with Implications for Cleavage by Secretases"

215. "Function of molecular chaperone GroEL follows the Iterative Annealing Mechanism", Physics Colloquium, Northeastern University, October 10, 2013.
216. "Noise suppression in a signaling cascade", 110th Statistical Mechanics meeting (celebration of 90th birthdays of Phil Anderson and Freeman Dyson) Rutgers University, Dec 16, 2013.

2014

217. "Towards a theory of molecular motors", GRC meeting on Protein Folding and Dynamics, Galveston, TX, January 8, 2014.
218. "Function of molecular chaperone GroEL follows the Iterative Annealing Mechanism", The 2nd International Symposium on Dynamical Ordering of Biomolecular Systems for Creation of Integrated Functions, Kyoto, Japan, January 12, 2014.
219. "Theory of motility of Myosin V", Department of Physics, Nagoya University, January 17, 2014.
220. "Theory of stepping and stomping of Myosin V", Duke University, February 24, 2014.
221. "Theory of motility of Myosin V", Muscle Institute, University of Pennsylvania, PA March 17, 2014.
222. "Role of water and membranes in amyloid formation", Department of Physics, University of Southern Florida, Tampa, FL, April, 11, 2014
223. "Stepping Kinetics of Myosin motors: Moving forward, backward, and foot stomping", Laufer center, Stony Brook University, NY April 22, 2014.
224. "Theory of Protein Folding" Summer School in "Active Systems", June 24, 2014, Gwang Ju, Korea.
225. "Theory of Molecular Machines" Summer School in "Active Systems", June 26, Gwang Ju, Korea.
226. "Crowding Promotes the switch from hairpin to pseudoknot conformation in human Telomerase RNA", Thematic meeting on "Significance of knotted Structures for function of proteins and Nucleic Acids", September 19, Warsaw, Poland.
227. "Design Principles Governing the motility of myosin V", 110th International Titisee Conference on "Structure, forces, and dynamics of macromolecular complexes", October 10, Titisee, Germany.

2015

228. "Design principles governing the motility of myosin V", Colloquium Temple University, Philadelphia, PA Feb 4, 2015.
229. "Design principles governing the motility of Myosin V", National Center for Biological Sciences, Bangalore, India, March 10, 2015.
230. "Design principles governing the motility of Myosin V", Department of Chemistry, University of Texas, Austin, May 4, 2015.
231. "Noise Control in a signaling network", NSF Workshop on "Physics of Wear, Tear, Aging, and Failure in Living and Non-Living systems", Hyatt Regency Tyson Corner, VA, May 08, 2015.
232. "Motility of Myosin V", 19th Conversation Albany, June 11, 2015.
233. "Design principles governing the motility of Myosin V", MIT, September 23, 2015.
234. "Helicase processivity not the unwinding velocity exhibits universal increase with Force", Arieh Warshel 75th Birthday Symposium: Multiscale Modeling of Complex Molecules and Life

Processes", University of Southern California, LA November, 21 2015.

2016

238. "Architectural basis of stepping of Myosin" Chemical Research Society of India, February, 6 2016, Chandigarh, India.
239. "Design principles governing the motility of Myosin V", Physics Colloquium, Boston College, MA, February 24, 2016.
240. "Response of Proteins to force", APS meeting, Baltimore, March 18, 2016.
241. "Architectural basis of stepping of Myosin", Department of Chemistry, Yale University, April 12, 2016.
242. "Architectural basis of stepping of Myosin", Department of Biophysics, Wesleyan University, April 30, Middleton, CT (2016).
243. "How does Mg ions direct Ribozyme Folding", Meeting "Energy Landscapes: From Protein folding to Molecular Assembly", Sante Fe, May 11, 2016.
244. "RNA and Protein Folding: Spontaneous and Assisted", July 11, N. Cabrera Summer School: The Physics of Biological Systems: From Biomolecular nanomachines to Tissues and Organisms.
245. "Architectural basis of motility of Motors", July 12, , N. Cabrera Summer School: The Physics of Biological Systems: From Biomolecular nanomachines to Tissues and Organisms.
246. "How do metal ions direct ribozyme folding", **Award Lecture,** August 23, ACS Meeting Philadelphia.
247. "Crowding effects on Intrinsically Disordered Proteins", August 23, ACS Meeting, Philadelphia.
248. "Architectural Basis of the motility of Myosin V", **Physics Colloquium**, September 21, University of Illinois at Chicago.
249. "GroEl rescues substrate proteins by an Iterative Annealing Mechanism", September 22, University of Illinois, at Chicago.
250. "Architectural Basis of the motility of Myosin V", **Plenary Speaker,** Third International Conference on Computational Science and Engineering, November, 29, Hoh Chi Min City, Vietnam.

2017

251. "Protein and RNA chaperones optimize the Rate of Native State Production by the Iterative Annealing Mechanism", February 12, Annual Biophysical Society Meeting, New Orleans, LA
252. "Understanding RNA folding", CECAM Workshop: Challenges across Large Scale Biomolecular and Polymer Simulations, February, 22Vienna, 2017.
253. "How do divalent cations control the folding of Group I Introns", **Keynote Speaker,** Texas Protein Folders & Function meeting, April 8, Cleveland, TX 2017.
254. "Design principles governing the motility of Myosin Motors", April 18, Center for Theoretical and Biological Physics, Rice University, Houston.
255. "How do Ribozymes Fold?", May 1, Department of Chemistry, University of California, Riverside, CA.
256. "Motility of Myosin motors", May 2, Department of Chemistry, University of California, Irvine, CA.
257. "Theory of motor motility", May 4, Covariance Analysis in Biology", Harvard University (Applied Mathematics), Cambridge, MA.

258. “Physical basis for tumor evolution and heterogeneity”, International Conference in Biological Physics, Rio de Janeiro, June 8, 2017.
259. “Symmetry, rigidity, and Allosteric wiring diagram in multi-domain proteins”, Royal Society Symposium, London, June 19, 2017.
260. “Is there a role for theory and computations in Biology”, Telluride Summer School, July 24, 2017.
261. “Upward Curvature in force-dependent unfolding rate implies parallel unfolding”, Cambridge University, Jane Clarke Symposium, September 7, 2017.
262. “Physical basis for tumor evolution and heterogeneity”, Colloquium, Cancer Center, University of Pennsylvania, PA, September 25, 2017.
263. “Coarse-Grained and Minimal Models: Methodology and Applications”, International Meeting, UNAM University, Mexico City, Mexico, October 12, 2017.
264. “Motility of Myosin Motors”, Harvard University, Shakhnovich Symposium, December 6, 2017.

2018

265. “Force-dependent Velocity distribution in Motors”, Rice University, Onuchic Symposium, January 5, 2018.
266. “On the Universality of Collapse of Polypeptide Chains”, GRC meeting “Protein folding Dynamics”, Galveston, TX January 9, 2018.
267. “Organization and Dynamics of Chromosomes”, National Institutes of Health (NIDDK), February, 8, 2018.
268. “Organization and Dynamics of Chromosomes”, Department of Chemistry, UCLA, March 5, 2018
269. “Organization and Dynamics of Chromosomes”, Department of Chemistry, Material Research Laboratory, UCSB March, 14, 2018.
270. “Architectural Basis of the motility of Myosin V”, Department of Physics, Arizona State University, March 28, 2018.
271. “Organization and Dynamics of Chromosomes”, Department of Chemistry, MIT, April 10, 2018.
272. “Out of Equilibrium glassy dynamics of Interphase Chromosomes”, Biophysics Symposium in Honor of Geroge H. Lorimer, University of Maryland, College Park, May, 11 2018.
273. “Out of Equilibrium glassy dynamics of Interphase Chromosomes”, Weizmann Institute, Rehovat, Israel, July 15, 2018.
274. “Architectural Basis of the motility of Myosin V”, Weizmann Institute, Rehovat, Israel, July 17, 2018.
275. “Out of Equilibrium glassy dynamics of Interphase Chromosomes”, Hebrew University Jerusalem, Israel, July 18, 2018.
276. “Interphase human chromosome exhibits out of equilibrium glassy dynamics”, Statistical Physics in Biology – Symposium in honor of Ken Dill – Arizona State University, October 8, 2018.
277. “Symmetry, Rigidity, and Allosteric Wiring Diagram in Multidomain Proteins”, CECAM-Lugano, Switzerland, October 18, 2018.
278. “Is there a role for theory and computations in biology”, University of Cincinnati, Oesper Symposium Award, November 9, 2018.
279. “From Caging to Super Diffusive Behavior in Tumor Growth”, Simon Foundation Symposium on Non-equilibrium processes in Biology, December 5, 2018

2019

280. “From glass-like to Super Diffusive behavior in Timor Growth”, National Institutes of Health (NIDDK), January 30, 2019.
281. “Interphase Human Chromosome Exhibits Glassy Dynamics”, March 5, 2019, Award Lecture, American Physical Society, Boston, MA.
282. “Interphase Human Chromosome Exhibits Glassy Dynamics”, Laufer Center, Stony Brook University, March 15, 2019.
283. “Interphase Human Chromosome Exhibits Glassy Dynamics”, University of North Texas, March 22, 2019
284. “Theory of Molecular Motors”, Johns Hopkins University, March 27, 2019
285. “Role of Diffusion in the Stepping Kinetics of Molecular Motors”, Conference: Nuclear and Cytoplasmic Machines at work, NYU, Abu Dhabi, April 9, 2019.
286. “Role of water in protein aggregation and amyloid polymorphism”, Workshop: Integrative Approaches to Protein Folding and Aggregation, Lisboa, Portugal, June 12, 2019.
287. “GroEL and RNA Chaperones as Active Stochastic Machines: A Unified Theory”, Award Address, 33rd annual Protein Society Meeting, July 1, 2019
288. “Interphase Human Chromosome Exhibits Glassy Dynamics”, Genome Architecture and Dynamics, July 15, 2019 Varna, Bulgaria.
289. “Role of water in protein aggregation and amyloid polymorphism”, GRC Meeting – Physics and chemistry of Liquids, Holderness School, New Hampshire, August 8, 2019.
290. “From Glass to super-diffusion in an evolving cell colony”, 40 Years of Replica Symmetry Breaking, Spienza Universita Di Roma, September 12, 2019.
291. “Glass-like Dynamics in Interphase Chromosomes”, Conference on 4D Epigenome, Venice Italy, October 5, 2019
292. ”Cell growth rate dictates glass to fluid-like transition and long time super diffusion in an evolving cell colony”, Cell Physics 2019, Saarbruckern, Germany, October 10, 2019.
293. “Role of water in protein aggregation and Amyloid Polymorphism”, International conference on Pathomechanisms of Amyloid Diseases, Maiami, Florida, December 19, 2019.