

## Ronald M. Levy

Laura H. Carnell Professor, Temple University

### Education

Reed College, Portland, OR	Biology/Mathematics	A.B. (1970)
Harvard University, Cambridge, MA	Biophysics	Ph.D. (1976)
Harvard University, Cambridge, MA	Chemistry	Post-Doc (1976-80)

### Professional Appointments

2014-	Professor of Chemistry (primary appointment), Physics, Biology, Temple University
2005-2012	Director, BioMaPS Institute for Quantitative Biology, Rutgers University
2004-2013	Adjunct Professor, Biochemistry, Robert Wood Johnson Medical School, UMDNJ
2002-2013	Board of Governors Professor of Chemistry and Chemical Biology, Rutgers University
2002-2005	Co-Director, BioMaPS Institute for Quantitative Biology, Rutgers University
1991-2002	Professor II, Chemistry, Rutgers University
1987-91	Professor, Chemistry, Rutgers University
1986	Visiting Professor, Crystallography Laboratory, CNRS, Strasbourg (France)
1984-87	Associate Professor, Chemistry, Rutgers University
1980-84	Assistant Professor, Chemistry, Rutgers University

### Honors

Alfred P. Sloan Foundation Fellow (1982)  
NIH Research Career Development Award (1982)  
NIH Fogarty International Center Senior Fellowship (1986)  
Johnson and Johnson Discovery Research Award (1987)  
John Simon Guggenheim Foundation Fellowship (1995)  
Rutgers University Board of Trustees Award for Excellence in Research (1996)  
Japan Society for the Promotion of Science Fellowship (1996)  
Plenary Lecturer, Alan J. Perlis Symposium, Yale University, (1997)  
American Association for the Advancement of Science, Fellow (1998)  
Board of Governors Professor of Chemistry and Chemical Biology, Rutgers University (2002)  
Keynote Speaker, "Alliance for Bioinformatics and Computational Biology", Texas Tech (2009)  
Keynote Speaker, "From Computational Biophysics to Systems Biology", U. Tennessee (2012)  
Laura H. Carnell Professor, Temple University (2014)  
Festschrift Issue of Protein Science to honor the career and 65<sup>th</sup> birthday of R.M. Levy (2016)

### Professional activities, selected

Associate Editor, Protein Science (1994-1997; 2011-present)  
Editorial Board, Journal of Chemical Theory and Computation (ACS), (2004- 2013)  
Co-Editor, Current Opinion in Structural Biology, Theory & Computation (1998, 2000, 2017)  
NIH Study Sections (term member 1991-1995, 2002, 2004, 2005, 2008, 2012, term member 2015-2021)  
NAS, Committee to Evaluate Proposals for the Study of Molecular Dynamics on Anton (2010)  
Executive Committee, American Chemical Society, Physical Chemistry Division (1997-00)  
Executive Committee, American Physical Society, Division of Computational Physics (2007-10)  
Organizer, American Chemical Society National Meeting Symposia in 2000, 2004, 2014, 2016  
Advisory Boards: Schrödinger Inc. (1995-present); NIH Research Resource--Biological Magnetic Resonance Databank (University of Wisconsin, Madison) (1997-2003); Center for Biological Modeling, Michigan State University (2001-2005); University of Pittsburgh School of Medicine Center for Computational Biology and Bioinformatics (2003-2005); Japan Ministry of Science & Technology Priority Research Area "Physical Forces Affecting Protein Folding and Misfolding" (2004-2008).

### Contributions to Science

Levy is a founding member and pioneer among the group of scientists who developed molecular dynamics simulations of proteins into the powerful technique widely used in chemistry, biophysics, and structural biology that it is today. He was the first to connect molecular simulations of proteins with Nuclear Magnetic Resonance relaxation experiments, and the first to carry out simulations of a protein under high pressure. Using computational statistical mechanics as a framework, he has been a leader in studying solvation effects in chemistry and biophysics, and in developing methods

and effective potentials for simulating these systems. Levy has developed novel approaches to study protein kinetics on very long time scales by combining replica exchange simulations with Markov State Models. His studies of protein-ligand binding have emphasized the importance of entropic effects, as exemplified by the binding of ligands to Cytochrome P450s and other proteins. In his current research, Levy is using evolutionary Potts Hamiltonian models to study the fitness and free energy landscapes which control protein allostery.

#### **Ten Publications (selected from 200, H-index 62)**

Lipari, G., A. Szabo, and R.M. Levy. Protein Dynamics and NMR Relaxation: Comparison of Simulations with Experiments. *Nature*, 300, 197-198 (1982)

Kitchen, D.B., L.H. Reed, and R.M. Levy. Molecular Dynamics Simulation of Solvated Protein at High Pressure. *Biochemistry*, 31, 10083-10093 (1992)

Levy, R.M., and E. Gallicchio. Computer Simulations with Explicit Solvent: Recent Progress in the Thermodynamic Decomposition of Free Energies, and in Modeling Electrostatic Effects. *Annual Review of Physical Chemistry*, 49, 531-567 (1998)

Murphy, L.R., A. Wallqvist, and R.M. Levy. Simplified Amino Acid Alphabets for Protein Fold Recognition and Implications for Folding. *Prot. Eng.*, 13, 149-152 (2000)

Andrec, M., A.K. Felts, E. Gallicchio, and R.M. Levy. Protein Folding Pathways from Replica Exchange Simulations and a Kinetic Network Model. *Proc. Natl. Acad. Sci. USA*, 102, 6801-6806 (2005)

Ravindranathan, K.P., E. Gallicchio, R.A. Friesner, A.E. McDermott, and R.M. Levy. Conformational Equilibrium of Cytochrome P450 BM-3 Complexed with N-Palmitoylglycine: A Replica Exchange Molecular Dynamics Study. *J. Am. Chem. Soc.*, 128, 5786-5791 (2006)

Lapelosa, M., E. Gallicchio, G. Ferstandig Arnold, E. Arnold, and R.M. Levy. In silico vaccine design based on molecular simulations of rhinovirus chimeras presenting HIV-1 gp41 epitopes. *J. Mol. Biol.*, 385, 675-691 (2009), PMID: PMC2649764. doi:10.1016/j.jmb.2008.10.089

Gallicchio, E., M. Lapelosa, and R.M. Levy. The Binding Energy Distribution Analysis Method (BEDAM) for the Estimation of Protein-Ligand Binding Affinities. *J. Chem. Theory Comput.*, 6, 2961-2977 (2010) PMID: PMC2992355. doi:10.1021/ct1002913

Dai, W., A. Sengupta, and R. M. Levy. First Passage Times, Lifetimes, and Relaxation Times of Unfolded Proteins. *Physical Review Letters*, 115 (4), 048101-048105 (2015) . doi:10.1103/PRL.115.048101, PMID: PMC4531052

Haldane, Allan, William F. William, Peng He, R. S. K. Vijayan, and Ronald M. Levy (2016). Structural propensities of kinase family proteins from a Potts model of residue co-variation. *Protein Science*, 25 (8), 1378–1384. doi: 10.1002/pro.2954

#### **Graduate and Postdoctoral Advisors:**

Graduate advisor: Martin Kushmerick, Harvard University

Postdoctoral advisor: Martin Karplus, Harvard University

#### **Graduate and Post Doctoral Scholars Sponsored (17 PhD students, 26 postgraduate scholars)**

##### **PhD Students over last 5 years** (with current affiliation)

Weihua Zheng (Rice University); Chitra Narayanan (U. of Toronto); William Flynn (Temple University); Kristina Paris (University of Pittsburgh); Omar Haq (World Quant); Wei Dai (Bloomberg Financial); Mauro Lapelosa (Genentech); Peng He (Temple University)

##### **Postgraduate-Scholar Sponsor over last 5 years** (with current affiliation)

Dr. Ahmet Mentesh (University of Pennsylvania); Dr. Di Cui (Temple University); Dr. Allan Haldane (Temple University); Dr. Robert Harris (University of Maryland); Dr. Vijayan Ramaswamy (M.D. Anderson Medical Center); Dr. Emilio Gallicchio (Brooklyn College, CUNY); Dr. Nanjie Deng (Pace University)