

Robert H. Havlin, Ph.D.

Postdoctoral Chemist
National Institutes of Health
Laboratory of Chemical Physics
National Institute of Diabetes and Digestive and Kidney Diseases
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Education:

Ph.D., Physical Chemistry , University of California, Berkeley,	2002
Dissertation Title: "Utilizing Dipolar Couplings for Structure Determination in Solutions, Solids, and Liquid Crystals." Advisor: Professor Alex Pines	
B.S., Chemistry, highest distinction , University of Illinois, Urbana-Champaign	1997
Thesis Title: "Solid State NMR and Quantum Mechanical Calculations of NMR Spectroscopic Parameters." Advisor: Professor Eric Oldfield	

Research Interests:

Postdoctoral: 'Snapshots of Protein Folding': Developed a nuclear magnetic resonance (NMR) method for elucidating protein folding intermediates in frozen solutions utilizing solid state NMR. Observed unfolding processes in the helical subdomain of the protein villin. Improved the understanding of vitally important protein folding events with the use of quantum chemical computational methods. Future exploration of this subject will provide detailed insight into enzyme activity as well as inhibitory action of drug targets for diseases such as HIV.

Doctoral: Developed novel NMR methodologies for the study of dipolar couplings in oriented liquid crystalline samples for structure determination. Utilized the chemical shift anisotropy tensor for structure prediction of proteins in the solid and liquid state.

Undergraduate: Effectively pushed the limits of existing quantum mechanical methods for structure determination in a variety of systems using several spectroscopic techniques including NMR and Mössbauer spectroscopy.

Grants, Scholarships and Fellowships:

Burroughs Wellcome Career Award at the Scientific Interface	(\$500,000)	(2005)
National Science Foundation Graduate Fellowship		(1997)
Procter and Gamble Research Award		(1997)
Bailar Undergraduate Research Scholarship		(1997)
Barry M. Goldwater Scholarship		(1996)
Clarence Brehm Scholarship		(1996)
Bloom Scholarship		(1996)
Peter C. and Gretchen Miller Markunas Scholarship Award		(1995)
PPG Industries Research Fellowship		(1994)

Honors:

Fellows Award for Research Excellence (NIH)	(2006)
Marvel Research Award	(1997)
Rodebush Award	(1997)
Colgate-Palmolive Research Award	(1995)
Arthur Sloan Prize	(1995)

Professional Associations:

American Chemical Society
American Association for the Advancement of Science
Biophysical Society

Professional Experience:

Reviewer: Journal of the American Chemical Society	(2003-)
Journal of Biomolecular NMR	
Journal of Physical Chemistry	
Faculty, Foundation for Advanced Education in Science, NIH, Bethesda, MD	(2004-)
Graduate Introductory Biophysics	
Postdoctoral Chemist, National Institutes of Health, Bethesda, MD	(2003-)
Laboratory of Chemical Physics, NIDDK	
Graduate Research Assistant, U.C. Berkeley, Berkeley CA	(1997 – 2002)
Graduate Student Instructor, U.C. Berkeley, Berkeley CA	
<i>Chemistry 98B: Order, Disorder, and Chaos</i>	(Spring 2001)
<i>Chemistry 130A: Biophysical Chemistry</i>	(Spring 1999)
<i>Chemistry 1A: General Chemistry</i>	(Fall 1997)
Research Assistant in Physical Chemistry, University of Illinois – Urbana, IL	(1993 – 1997)
Teaching Assistant in Physical Chemistry, University of Illinois – Urbana, IL	
<i>Chemistry 342: Physical Chemistry, I</i>	(1996)
<i>Chemistry 345: Physical Principles of Chemistry Laboratory, I</i>	(1997)

Publications:

21. **R. H. Havlin** and R. Tycko, *Proc. Natl. Acad. Sci.* 102 (9): 3284-3289 (2005). Probing site-specific conformational distributions in protein folding with solid state NMR.
20. **R. H. Havlin**, J.D. Walls, A. Pines, *J. Chem. Phys* 122: 074507 (12pgs.) (2005). Isotropic Proton-detected Local-field Nuclear Magnetic Resonance in Solids.
19. **R. H. Havlin**, G.H.J. Park, T. Mazur, A. Pines, *J. Am. Chem. Soc.* **125**(26): 7998-8006 (2003). Using switched angle spinning to simplify NMR spectra of strongly oriented samples.
18. M. Marjanska, **R. H. Havlin**, D. Sakellariou, Coherent Averaging and Correlations of Anisotropic Spin Interactions in Oriented Molecules, in *NMR of Ordered Liquids*, E.E. Burnell and C.A. De Lange, Editors. 2003, Kluwer Academic. p. 455.
17. J.D. Walls, W.B. Blanton, **R. H. Havlin**, A. Pines, *Chem. Phys. Lett.* **363**(4): 372-380 (2002). Creating Isotropic Dipolar Spectra for a Pair of Dipole Coupled Spins in High-field.
16. **R. H. Havlin**, G.H.J. Park, A.Pines, *J. Magn. Reson.* **157**: 163-169 (2002). Two Dimensional NMR Correlations of Liquid Crystals Using Switched Angle Spinning.
15. **R. H. Havlin**, D. D. Laws, H. M. L. Bitter, L. K. Sanders, H. Sun, J. S. Grimley, D. E. Wemmer,

- A. Pines, and E. Oldfield, *J. Am. Chem. Soc.* **123**(42): 10362-10369 (2001). An Experimental and Theoretical Investigation of the Chemical Shielding Tensors of ^{13}C of Alanine, Valine, and Leucine Residues in Solid Peptides and in Proteins in Solution
14. Godbout N, Sanders LK, Salzmann R, **R. H. Havlin**, Wojdelski M, Oldfield E, *J. Am. Chem. Soc.* **121**: 3829-3844 (1999). Solid-state NMR, Mössbauer, crystallographic, and density functional theory investigation of Fe-O₂ and Fe-O₂ analogue metalloporphyrins and metalloproteins.
13. M. Tomaselli , J.L. Yarger , M. Bruchez, **R. H. Havlin**, D. deGraw, A. Pines, A.P. Alivisatos, *J. Chem. Phys.* **110**(18): 8861-8864 (1999). NMR study of InP quantum dots: Surface structure and size effects.
12. M. McMahon, A. C. de Dios, N. Godbout, R. Salzmann, D. D. Laws, H. Le, **R. H. Havlin**, and E. Oldfield, *J. Am. Chem. Soc.* **120**(19): 4784-4797 (1998). An experimental and quantum chemical investigation of CO binding to heme proteins and model systems: A unified model based on ^{13}C , ^{17}O , ^{57}Fe nuclear magnetic resonance, ^{57}Fe Mössbauer and infra-red spectroscopy.
11. Haake M., Goodson B.M., Laws D.D., Brunner E., Cyrier M.C., **R. H. Havlin**, Pines A., *Chem. Phys. Lett.* **292**: 686-690 (1998). NMR of supercritical laser-polarized xenon.
10. N. Godbout, **R. H. Havlin**, R. Salzmann, M. Wojdelski, P. G. Debrunner and E. Oldfield, *J. Phys. Chem. A* **102**(13): 2342-2350 (1998). Iron-57 NMR chemical shifts and Mössbauer quadrupole splittings in ferrocytocchrome c and myoglobins: A density functional investigation.
9. R. Salzmann, M. Wojdelski, M. McMahon, **R. H. Havlin** and E. Oldfield, *J. Am. Chem. Soc.* **120**(7): 1349-1356 (1998). A solid-state nitrogen-15 nuclear magnetic resonance spectroscopic and quantum chemical investigation of nitrosoarene-metal interactions in model systems and in heme proteins.
8. **R. H. Havlin**, N. Godbout, R. Salzmann, M. Wojdelski, W. Arnold, C. E. Schulz and E. Oldfield, *J. Am. Chem. Soc.* **120**(13): 3144-3151 (1998). An experimental and density functional theoretical investigation of iron-57 Mössbauer quadrupole splittings in organometallic and heme-model compounds: Applications to heme protein structure.
7. J. G. Pearson, H. Le, L. Sanders, N. Godbout, **R. H. Havlin** and E. Oldfield, *J. Am. Chem. Soc.* **119**(49): 11941-11950 (1997). Predicting chemical shifts in proteins: Structure refinement of valine residues by using *ab initio* and empirical geometry optimizations.
6. **R. H. Havlin**, H. Le, D. D. Laws, A. C. de Dios and E. Oldfield, *J. Am. Chem. Soc.* **119**(49): 11951-11958 (1997). An *ab initio* quantum chemical investigation of ^{13}C NMR shielding tensors in glycine, alanine, valine, isoleucine, serine, and threonine: comparisons between helical and sheet tensors, and the effects of c_1 on shielding.
5. **R. H. Havlin**, M. McMahon, R. Srinivasan, H. Le and E. Oldfield, *J. Phys. Chem. A* **101**(47): 8908-8913 (1997). A solid state NMR and density functional investigation of ^{13}C shielding tensors in metal-olefin complexes.
4. J. Heller, D. D. Laws, D. S. King, A. Pines, D. E. Wemmer, **R. H. Havlin**, and E. Oldfield, *J. Am. Chem. Soc.* **119**: 7827-7831 (1997). Determination of Dihedral Angles in Peptides Through Experimental and Theoretical Studies of Alpha Carbon Chemical Shielding Tensors.
3. J. Feeney, J. E. McCormick, C. J. Bauer, B. Birdsall, C. M. Moody, B. A. Starkmann, D. W. Young, P. Francis, **R. H. Havlin**, W. D. Arnold, and E. Oldfield, *J. Am. Chem. Soc.* **118**: 8700-8706 (1996). Fluorine-19 Nuclear Magnetic Resonance Chemical Shifts of Fluorine Containing Aliphatic Amino Acids in Proteins: Studies of *Lactobacillus casei* Dihydrofolate Reductase Containing (2S,4S)-5-Fluoroleucine.
2. D. D. Laws, H. Le, A. C. de Dios, **R. H. Havlin**, and E. Oldfield, *J. Am. Chem. Soc.*, **117**, 9542-9546 (1995). A Basis Size Dependence Study of ^{13}C Nuclear Magnetic Resonance Spectroscopic Shielding in Alanyl and Valyl Fragments: Toward Protein Shielding Hypersurfaces.
1. D. D. Laws, D. S. Wishart, **R. H. Havlin**, M. Westmeyer, B. D. Sykes and E. Oldfield, *J. Magn. Reson., B*, **108**, 274-275 (1995). $\text{N},\text{N}',\text{N}''$ -Trimethyl(2-trimethylsilyl)ethylammonium Iodide: A Universal Internal Standard for ^1H , ^{13}C , and ^{15}N NMR.

Oral Presentations (Invited):

1. **R. H. Havlin**, R. Tycko "Snapshots of Protein Folding: Elucidating 'freeze-trapped' Intermediates with Solid State NMR," Georgetown University Department of Chemistry Seminar, Washington, DC, April 7, 2005.
2. **R. H. Havlin**, R. Tycko "Probing Site Specific Conformational Distributions in Proteins with Solid State NMR," NIH Structural Biology Interest Group Seminar, Bethesda, MD, January 12, 2005.
3. **R. H. Havlin**, R. Tycko, "Unraveling Protein Folding with Site Specific Conformational Detail," 45th Experimental NMR Conference, Asilomar, CA, April 20, 2004.
4. **R. H. Havlin**, R. Tycko, "Snapshots of Folding in the Small Helical Protein, HP35," Protein Folding Interest Group Seminar, Bethesda, MD, November 12, 2003.
5. **R. H. Havlin**, J.D. Walls, W.B. Blanton, A. Pines, "Dipolar Couplings in Solids: Measurement and Assignment Using Novel Techniques," 44th Rocky Mountain Conference Symposium on NMR, Denver, CO, July 28 – August 1, 2002.
6. **R. H. Havlin**, W.B. Blanton, J.D. Walls, T. Mazur, K.L. Pierce, A. Pines, "Creating Isotropic Dipolar Spectra," 30th Congress Ampere on Magnetic Resonance and Related Phenomena, Lisbon, Portugal, July 23, 2000.
7. **R. H. Havlin**, R. Salzmann, N. Godbout, M.T. McMahon, L.K. Sanders, C.M. Szabo, E. Oldfield, "Solid State NMR of Proteins and Model Systems: Experimental and Theoretical Approaches," American Chemical Society 214th National Meeting, Las Vegas, NV, September 10, 1997.
8. **R. H. Havlin**, R. Salzmann, N. Godbout, M.T. McMahon, E. Oldfield, "Heme Protein Ligand Structure Via NMR," Procter and Gamble - Chemistry at Illinois, Urbana, IL, March 18, 1997.