

## Curriculum Vitae

Name: Sherwin Singer  
Title: Professor

Born: March 20, 1954  
Department: Chemistry

### Education

<i>Institution (Preceptor)</i>	<i>Degree</i>	<i>Date</i>	<i>Field</i>
University of Chicago	A.B.	1976	Chemistry
Princeton University	–	1976-1978	History of Science
University of Chicago (Karl F. Freed)	Ph.D.	1984	Chemistry
University of Pennsylvania (David Chandler)	postdoc	1983-1985	Chemistry
AT&T Bell Laboratories (John D. Weeks)	postdoc	1985-1986	Chemistry

### Positions/Research Experience

<i>Institution</i>	<i>Position</i>	<i>Dates</i>	<i>Activities</i>
Ohio State University	Assistant Professor	1/87-9/93	Teaching/Research
Ohio State University	Associate Professor	10/93-9/03	Teaching/Research
Ohio State University	Professor	10/03-	Teaching/Research

### Honors

National Science Foundation Predoctoral Fellow	1977
Camille and Henry Dreyfus Foundation Distinguished New Faculty	1985
Dozor Fellowship, Ben-Gurion University, Beer Sheva, Israel	1998

### Research Interests

Statistical mechanics; phase transitions in molecular fluids and solids, surfactant solutions and monolayers; biomolecular transport in nanochannels; classical and quantum dynamics in condensed phases, clusters, and biological systems.

### Publications

1. R. Hsu, S. J. Singer, P. Keim, T. F. Deuel, and R. L. Heinrikson, "Structural studies of *Bacillus subtilis* glutamine synthetase: further purification, sulfhydryl groups, and the amino-terminal amino acid sequence", *Arch. Biochem. Biophys.* **178**:644 (1977).
2. S. J. Singer, K. F. Freed and Y. B. Band, "Electronic angular momentum effects on photodissociation: fine structure cross sections and angular distributions for  $\text{NaH} \rightarrow \text{Na}(^2P_{1/2,3/2}) + \text{H}(^2S_{1/2})$ ", *Chem. Phys. Lett.* **91**:12 (1982).

3. S. J. Singer, K. F. Freed and Y. B. Band, "Invariant imbedding solution of driven (inhomogeneous) Schrodinger equations", *J. Chem. Phys.* **77**:1942 (1982).
4. S. J. Singer, K. F. Freed and Y. B. Band, "Theory of diatomic molecule photodissociation: electronic angular momentum influence on fragment cross sections", *J. Chem. Phys.* **79**:6060 (1983).
5. S. J. Singer, K. F. Freed and Y. B. Band, "Electronic energy partitioning in photodissociation", in *Laser Chemistry* **3**:57 (Gordon and Breach, New York, 1983).
6. B. Bagchi, S. J. Singer and D. W. Oxtoby, "Non-monotonic dependence of electronic relaxation on solvent viscosity", *Chem. Phys. Lett.* **99**:225 (1983).
7. S. J. Singer, K. F. Freed and Y. B. Band, "Dissociation of a diatomic molecule to atomic fine structure states: electronically nonadiabatic effects upon resonant two-photon dissociation", *J. Chem. Phys.* **81**:3064 (1984).
8. S. J. Singer, K. F. Freed and Y. B. Band, "Cross sections and angular distributions for individual fragment fine structure levels produced in one- and two-photon photodissociation of NaH", *J. Chem. Phys.* **81**:3091 (1984).
9. S. J. Singer, K. F. Freed and Y. B. Band, "Low energy resonances in photodissociation of CH<sup>+</sup>", *Chem. Phys. Lett.* **105**:158 (1984).
10. W. S. Struve, S. J. Singer and K. F. Freed, "Photodissociation of homonuclear diatomics: fine structure cross sections for Na<sub>2</sub> → Na(<sup>2</sup>S<sub>1/2</sub>) + Na(<sup>2</sup>P<sub>1/2,3/2</sub>)", *Chem. Phys. Lett.* **110**:588 (1984).
11. S. J. Singer, K. F. Freed and Y. B. Band, "Photodissociation of diatomic molecules to open shell fragments", *Adv. Chem. Phys.* **61**:1 (1985).
12. S. J. Singer and D. Chandler, "Free energy functions in the extended RISM approximation", *Mol. Phys.* **55**:621 (1985).
13. Y. B. Band, K. F. Freed and S. J. Singer, "Orientation, alignment, and hyperfine effects on dissociation of diatomic molecules to open shell atoms", *J. Chem. Phys.* **84**:3762 (1986).
14. D. Chandler, J. D. McCoy and S. J. Singer, "Density functional theory of nonuniform polyatomic systems. I. General Formulation", *J. Chem. Phys.* **85**:5971 (1986).
15. D. Chandler, J. D. McCoy and S. J. Singer, "Density functional theory of nonuniform polyatomic systems. II. Rational closures for integral equations", *J. Chem. Phys.* **85**:5977 (1986).

16. S. J. Singer, R. A. Kuharski and D. Chandler, "RISM calculation of the activation barrier for isomerization of solvated cyclohexane", *J. Phys. Chem.* **90**:6015 (1986).
17. F. H. Mies, P. S. Julienne, Y. B. Band and S. J. Singer, "A convergent analysis of radiative matrix elements in atomic lineshape theory", *J. Phys.* **B19**:3249 (1986).
18. C. J. Williams, K. F. Freed, S. J. Singer and Y. B. Band, "Nonadiabatic effects on the photodissociation of diatomic molecules to open-shell atoms", *Faraday Disc. Chem. Soc.* **82**:51 (1986).
19. S. J. Singer and J. D. Weeks, "Renormalized finite cluster expansions", *Phys. Rev.* **B36**:2228 (1987).
20. Sherwin J. Singer, Sungyul Lee, Karl F. Freed, and Yehuda B. Band, "Multichannel quantum theory for propagation of second order transition amplitudes", *J. Chem. Phys.*, **87**, 4762, (1987).
21. J. D. McCoy, S. J. Singer and D. Chandler, "A density functional treatment of the hard dumbbell freezing transition", *J. Chem. Phys.* **87**:4853 (1987).
22. Yehuda B. Band, Karl F. Freed, Sherwin J. Singer, and Carl J. Williams, "Nonadiabatic effects on the photodissociation of diatomic molecules to open-shell atoms", *J. Phys. Chem.*, **91**, 5402, (1987).
23. R. A. Kuharski, D. Chandler, J. A. Montgomery, Jr., F. Rabii, and S. J. Singer, "Stochastic molecular dynamics study of cyclohexane isomerization", *J. Phys. Chem.* **92**:3261 (1988).
24. Sherwin J. Singer, Sungyul Lee, and Karl F. Freed, "Incorporating advantages of time-dependent dynamics in time-independent collision methods: early asymptotic analysis", *J. Chem. Phys.*, **91**, 240, (1989).
25. Sherwin J. Singer, "Multiparticle Monte Carlo moves: algorithm for solids with free-energy determination", *Computer Physics Communications*, **59**, 463, (1990).
26. Sherwin J. Singer and Ruth Mumaugh, "Monte Carlo study of fluid-plastic crystal coexistence in hard dumbbells", *J. Chem. Phys.*, **93**, 1278, (1990).
27. Chiachin Tsou, Dario A. Estrin, and Sherwin J. Singer, "Electronic energy shifts of a sodium atom in argon clusters by simulated annealing", *J. Chem. Phys.*, **93**, 7187 (1990).
28. Dario A. Estrin, Chiachin Tsou, and Sherwin J. Singer, "Multiconfigurational electronic wave functions without a reference configuration: analysis of a simulated annealing strategy", *J. Chem. Phys.*, **93**, 7201, (1990).

29. C. H. Martin and S. J. Singer, "The behavior of point defects in a model crystal near melting", *Phys. Rev.* **B44**: 477 (1991).
30. D. A. Estrin, C. Tsao and S. J. Singer, "Accurate non-local electron-argon pseudopotential for condensed phase simulation", *Chem. Phys. Lett.* **184**: 571 (1991).
31. M. M. Hurley and S. J. Singer, "Domain energies of the dipolar lattice gas", *J. Phys. Chem.* **96**: 1938 (1992).
32. M. M. Hurley and S. J. Singer, "Phase transitions at zero temperature in the dipolar lattice gas", *J. Phys. Chem.* **96**: 1951 (1992).
33. C. Tsao, D. A. Estrin and S. J. Singer, "Electronic spectra of  $\text{NaAr}_4$  and  $\text{NaAr}_6$ : isomerization and melting", *J. Chem. Phys.* **96**: 7977 (1992).
34. D. A. Estrin, L. Liu and S. J. Singer, "Is  $\text{AlAr}_{12}$  icosahedral?" *J. Phys. Chem.* **96**: 5325 (1992).
35. M. M. Hurley and S. J. Singer, "Domain structure and phase transitions in the dipolar lattice gas", *Phys. Rev.* **B46**:5783 (1992).
36. Sherwin J. Singer, "Layer buckling in Smectic-A liquid crystals and two-dimensional stripe phases", *Phys. Rev.* **E48**:2796 (1993).
37. Karthik A. Iyer and Sherwin J. Singer, "Local mode analysis of complex zeolite vibrations: Sodalite", *J. Phys. Chem.* **98**:12670 (1994).
38. Karthik A. Iyer and Sherwin J. Singer, "Local mode analysis of complex zeolite vibrations: Zeolite-A", *J. Phys. Chem.* **98**: 12679 (1994).
39. Holly B. Lavender, Karthik A. Iyer and Sherwin J. Singer. "Global orientational order in model polar clusters", *J. Chem. Phys.* **101**: 7856 (1994).
40. Sherwin J. Singer, "Annealing to a moving target: first-principles molecular dynamics", in *Application of Simulated Annealing in Chemistry*, edited by John H. Kalivas (Elsevier, 1995).
41. Dongsheng Lu and Sherwin J. Singer, "Orientational ordering and anisotropy in model polar clusters", *J. Chem. Phys.* **103**: 1913 (1995).
42. Lars Ojamäe, Isaiah Shavitt and Sherwin J. Singer. "Potential energy surfaces and vibrational spectra of  $\text{H}_5\text{O}_2^+$  and larger hydrated proton complexes", *Int. J. Quantum Chem.* **29**: 657 (1995).
43. Dongsheng Lu and Sherwin J. Singer, "Ion solvation in model polar clusters", *J. Chem. Phys.* **105**: 3700 (1996).

44. R. E. Geer, S. J. Singer, J. V. Selinger, B. R. Ratna and R. Shashidhar, "Electric-field-induced layer buckling in chiral smectic-A liquid crystals", *Phys. Rev. E* **57**: 3059 (1998).
45. Shannon McDonald, Lars Ojamäe and Sherwin J. Singer, "Graph theoretical generation and analysis of hydrogen-bonded structures with applications to the neutral and protonated water cube and dodecahedral clusters", *J. Phys. Chem. A* **102**: 2824 (1998).
46. Lars Ojamäe, Isaiah Shavitt and Sherwin J. Singer, "An atom-atom potential for simulations of the solvated proton in water", *J. Chem. Phys.* **109**: 5547 (1998).
47. K. Rzążewski, M. Trippenbach, Y. B. Band and S. J. Singer, "Statistics of atomic populations in output-coupled wave packets from Bose-Einstein condensates: four-wave mixing", *Phys. Rev. A* **61**:013606 (1999).
48. Sherwin J. Singer, Shannon McDonald and Lars Ojamäe, "Topology vs. temperature: thermal behavior of  $\text{H}^+(\text{H}_2\text{O})_8$  and  $\text{H}^+(\text{H}_2\text{O})_{16}$ ", *J. Chem. Phys.* **112**(2):710 (2000).
49. Michael D. Tissandier, Sherwin J. Singer and James V. Coe, "Enumeration and evaluation of the water hexamer cage structure", *J. Phys. Chem.* **A104**(4):752 (2000).
50. Antitsa D. Stoycheva and Sherwin J. Singer, "Stripe melting in a two-dimensional system with competing interactions", *Phys. Rev. Lett.* **84**(20):4657 (2000).
51. Sherwin J. Singer, "Buckling induced by dilative strain in two- and three-dimensional layered materials", *Phys. Rev.* **E62**(3):3736 (2000).
52. Cristian V. Ciobanu, Lars Ojamäe, Isaiah Shavitt and Sherwin J. Singer, "Structure and vibrational spectra of  $\text{H}^+(\text{H}_2\text{O})_8$ : Is the excess proton in a symmetrical hydrogen bond?", *J. Chem. Phys.* **113**(13):5321 (2000).
53. Jer-Lai Kuo, James V. Coe, Sherwin J. Singer, Yehuda B. Band, and Lars Ojamäe, "On the use of graph invariants for efficiently generating hydrogen bond topologies and predicting physical properties of water clusters and ice", *J. Chem. Phys.* **114**(6):2527 (2001).
54. Antitsa D. Stoycheva and Sherwin J. Singer, "Scaling theory for two-dimensional systems with competing interactions", *Phys. Rev.* **E64**(1):16118 (2001).
55. Christopher Callam, Sherwin J. Singer, Todd L. Lowary, and Christopher M. Hadad, "Computational analysis of the potential energy surfaces of glycerol in the gas and

- aqueous phases. Effects of level of theory, basis set, and solvation on strongly intramolecularly hydrogen-bonded systems”, *J. Amer. Chem. Soc.* **123**(47):11743 (2001).
56. Antitsa D. Stoycheva and Sherwin J. Singer, “Computer simulations of a two-dimensional system with competing interactions”, *Phys. Rev.* **E65**(3):036706 (2002).
  57. Jer-Lai Kuo and Sherwin J. Singer, “ Graph invariants for periodic systems: predicting physical properties from the hydrogen bond topology of ice”, *Physical Review* **E67**(1):016114 (2003).
  58. Jer-Lai Kuo, Cristian V. Ciobanu, Lars Ojamäe, Isaiah Shavitt and Sherwin J. Singer, “Short H-Bonds and Spontaneous Self-Dissociation in  $(\text{H}_2\text{O})_{20}$ : Effects of H-Bond Topology”, *J. Chem. Phys.* **118**(8):2527 (2003).
  59. Xinchuan Huang, Hyung Min Cho, Stuart Carter, Lars Ojamäe, Joel M. Bowman, and Sherwin J. Singer, “Full Dimensional Quantum Calculations of Vibrational Energies of  $\text{H}_5\text{O}_2^+$ ”, *J. Phys. Chem.* **A107**(37):7142 (2003).
  60. Hyung Min Cho and Sherwin J. Singer, “Correlation function quantum Monte Carlo study of the excited vibrational states of  $\text{H}_5\text{O}_2^+$ ”, *J. Phys. Chem.* **A108**(41):8691 (2004) .
  61. Stephen D. Belair, Joseph S. Francisco and Sherwin J. Singer “Hydrogen bonding in cubic  $(\text{H}_2\text{O})_8$  and  $\text{OH} \cdot (\text{H}_2\text{O})_7$  clusters”, *Phys. Rev.* **A71**(1): 013204 (2005).
  62. Bruce C. Garrett, David A. Dixon, Donald M. Camaioni, Daniel M. Chipman, Mark A. Johnson, Charles D. Jonah, Gregory A. Kimmel, John H. Miller, Thomas N. Rescigno, Peter J. Rossky, Sotiris S. Xantheas, Steven D. Colson, Allan H. Laufer, Douglas Ray, Paul F. Barbara, David M. Bartels, Kurt H. Becker, Kit H. Bowen, Jr., Stephen E. Bradforth, Ian Carmichael, James V. Coe, L. Rene Corrales, James P. Cowin, Michel Dupuis, Kenneth B. Eisenthal, James A. Franz, Maciej S. Gutowski, Kenneth D. Jordan, Bruce D. Kay, Jay A. LaVerne, Sergei V. Lymar, Theodore E. Madey, C. William McCurdy, Dan Meisel, Shaul Mukamel, Anders R. Nilsson, Thomas M. Orlando, Nikolay G. Petrik, Simon M. Pimblott, James R. Rustad, Gregory K. Schenter, Sherwin J. Singer, Andrei Tokmakoff, Lai-Sheng Wang, Curt Wittig, and Timothy S. Zwier, “The Role of Water on Electron-Initiated Processes and Radical Chemistry: Issues and Scientific Advances”, *Chem. Rev.* **105**(1):355 (2005).
  63. Wei Zhu and Sherwin J. Singer, “Monte Carlo simulation of methyl chloride monolayer on the surface of graphite”, *Surf. Sci.* **579**(2-3):141 (2005).

64. Sherwin J. Singer, Jer-Lai Kuo, Tomas K. Hirsch, Chris Knight, Lars Ojame and Michael L. Klein, "Hydrogen bond topology and the ice VII/VIII and Ih/XI proton ordering phase transitions", *Phys.Rev.Lett.* (in press, 2005).
65. Wei Zhu, Sherwin J. Singer, Zhi Zheng and A. T. Conlisk, "Electroosmotic flow of a model electrolyte", *Phys. Rev. E* (in press, 2005).

### **Recent Invited Presentations 1996-2005**

- “Cluster Structure and Re-structuring Upon Solvation of Ionic and Non-ionic Solutes”, American Physical Society March Meeting, March 18-22, 1996, St.Louis, MO.
- “Stripes, Bubbles, Layers, and What Lies Between: Modulated Structures in Thin Films and Liquid Crystals”, Naval Research Lab, April 30, 1996, Washington, D.C.
- “Modulated Structures and Phase Transitions at Fluid Interfaces and Thin Films”, American Chemical Society Regional Meeting, June 9-12, 1996, Dayton OH.
- “Proton solvation in water clusters: quantum and classical Monte Carlo studies, graph theoretical enumeration of hydrogen-bonded arrangements, and compact/extended transitions”, American Chemical Society National Meeting, September 7-11, 1997, Las Vegas.
- “Stripes, Bubbles, Layers, and What Lies Between: Modulated Structures in Thin Films and Liquid Crystals”, Chemistry Department Colloquium at Carnegie Mellon University, October 21, 1997.
- “Stripes, Bubbles, Layers, and What Lies Between: Modulated Structures in Thin Films and Liquid Crystals”, Physical Chemistry Colloquium at Purdue University, November 5, 1997.
- “Proton solvation in water clusters”, Theoretical Chemistry Group Colloquium at Los Alamos National Labs, November 13, 1997.
- “Stripes, Bubbles, Layers, and What Lies Between: Modulated Structures in Thin Films and Liquid Crystals”, Chemistry Department Colloquium at University of New Mexico, November 14, 1997.
- “Stripes, Bubbles, Layers, and What Lies Between: Modulated Structures in Thin Films and Liquid Crystals”, Chemistry Department Colloquium at University of North Carolina and Chapel Hill, February 26, 1998.
- “Stripes, Bubbles, Layers, and What Lies Between: Modulated Structures in Thin Films and Liquid Crystals”, Chemistry Department Colloquium at Iowa State University, Ames, April 24, 1998.
- “Order and Complexity in Pattern Forming Systems”, Chemistry Department Colloquium, Ben-Gurion University, Beer Sheva, Israel, December 14, 1998.
- “Order and Complexity in Pattern Forming Systems”, Complex Fluid Seminar Series, Weizmann Institute, Rehovot, Israel, December 21, 1998



- “Order and Complexity in Pattern Forming Systems”, Physical Chemistry Colloquium, Hebrew University, Jerusalem, Israel, December 22, 1998.
- “Order and Complexity in Pattern Forming Systems”, Condensed Matter Colloquium, Department of Physics, Tel Aviv University, Tel Aviv, Israel, December 23, 1998.
- “H-Bond Topology in  $(\text{H}_2\text{O})_n$  and  $\text{H}^+(\text{H}_2\text{O})_n$ ”, Regional American Chemistry Society Meeting, Covington, KY, May 18, 2000.
- “H-Bond Topology in  $(\text{H}_2\text{O})_n$  and  $\text{H}^+(\text{H}_2\text{O})_n$ ”, Telluride workshop on *Water in Confined Geometries:  $\text{H}_2\text{O}$  Clusters, Particles, Surfaces and Thin Layers*, July 30-August 5, 2000.
- “Order and Complexity in Pattern Forming Systems”, International Symposium on Frontiers in Molecular Science 2002 (ISFMS2002), Qingdao, China, July 15-18, 2002.
- “Order and Complexity in Pattern Forming Systems”, Chemistry Colloquium, University of Tennessee, Knoxville, September 5, 2002.
- “New Perspectives on Water Clusters, Neutral and Protonated”, Workshop on Understanding the Role of Water on Electron-Initiated Processes and Radical Chemistry, Pacific Northwest National Laboratory, September 28-29, 2002.
- “New directions in the study of water in clusters, ice, and in nanochannels”, Symposium on Computational Chemistry, American Chemical Society Regional Meeting, Pittsburgh, PA, October 19 - 23, 2003.
- “Hydrogen bond order and disorder in ice”, Telluride Workshop on studies of ice, icy particles, ice surfaces, and ice-adsorbate interactions: a molecular view, July 25-30, 2004.
- “Hydrogen Bond Topology in Water Clusters and Ice”, Materials Science Lecture, McMaster University, October 6, 2004.
- “Order and Complexity in Pattern-Forming Systems”, Physics Department Colloquium, University of Waterloo, October 7, 2004.
- “Hydrogen Bond Topology in Water Clusters and Ice”, Chemistry Department Colloquium, University of Waterloo, October 8, 2004.
- “Hydrogen bond topology and proton ordering phase transitions in ice”, National American Chemistry Society Meeting, San Diego, March 13-17, 2005.

- (title to be announced) Pacificchem 2005 Symposium "Proton Transfer/Transport of H-bonded Liquids, Solids, Clusters and Interfaces", December 15-20 of 2005.

### Organization of Scientific Meetings

Gordon Research Conference on "Disorder in Materials", Chair for July 1998 meeting (and vice-Chair of 1996 meeting).

### Research Funding

## 1 Funded research as principal investigator

- *Freezing of diatomic molecules*  
*PI:* Sherwin J. Singer  
*Source:* Petroleum Research Fund - Type G  
*Project Location:* Ohio State University  
*Award Amount:* \$15,000.00  
*Award Dates:* 1987-1991
- *Electronic structure in dynamic environments*  
*PI:* Sherwin J. Singer  
*Source:* NSF-Chemistry  
*Project Location:* Ohio State University  
*Award Amount:* \$202,000.00  
*Award Dates:* 12/1/1991-11/30/1995
- *Order and complexity in pattern-forming systems*  
*PI:* Sherwin J. Singer  
*Source:* Petroleum Research Fund - Type AC  
*Project Location:* Ohio State University  
*Award Amount:* \$50,000.00  
*Award Dates:* 9/97-9/00
- *New directions in the study of ice and water clusters*  
*PI:* Sherwin J. Singer  
*Source:* NSF-Chemistry  
*Project Location:* Ohio State University  
*Award Amount:* \$270,000.00  
*Award Dates:* 8/01/01-7/31/05

Several proposals for computer resources were also funded at Ohio Supercomputer Center, Pittsburgh Supercomputer Center, and the Molecular Science Computing Facility at Pacific Northwest National Labs.

## 2 Funded research as co-investigator

- *Electronic structure in dynamic environments*  
*PI's:* Sherwin J. Singer and Sungyul Lee, Kyunghee University, Korea  
*Source:* NSF-International Programs (US/Korea)  
*Project Location:* Ohio State University  
*Award Amount:* \$9296  
*Award Dates:* 1993-1995
- *New numerical approaches to electron ionization*  
*PI's:* Sherwin J. Singer and C. William McCurdy, Lawrence Livermore Lab  
*Source:* NSF-Chemistry  
*Project Location:* Ohio State University  
*Award Amount:* \$57,000  
*Award Dates:* 1994
- *Engineered nanostructures for next-generation clinical chemistry*  
*PI's:* Michael Bissell, Terry Conlisk, Derek Hansford, Sherwin J. Singer  
*Source:* OSU Large Interdisciplinary Grant Development Program  
*Project Location:* Ohio State University  
*Award Amount:* \$125,000  
*Award Dates:* 1/1/05-12/31/06