CV of Max L. Berkowitz

EDUCATION:

1967-1972
Novosibirsk State University, USSR
Department of Physics, M.Sc.

1974-1978
Weizmann Institute of Science, Israel
Department of Physical Chemistry, Ph.D.

EXPERIENCE:

July 1983-present:
Assistant Professor, Associate Professor, Professor
Department of Chemistry, University of North Carolina, Chapel Hill, NC

Advanced Studies Institute in Molecular Dynamics, Jerusalem 1993, Visiting Scholar.

January 2001-March 2001 Visiting Professor, Department of Chemistry, UCLA

August, 1980-June, 1983; Visiting Assistant Professor
Department of Chemistry, University of Houston, Houston, TX

Nov., 1978-July, 1980: Postdoctoral Fellow
Department of Chemistry, Purdue University, West Lafayette, IN

AWARDS AND HONORS:

Prize for graduate work in Chemistry, 1978
Fellow of the American Physical Society, (1995)
W.Wiley Chair Professor , 1996-2001

RESEARCH INTERESTS:

Structural and dynamical properties of biomembranes, structure of lipid rafts, interaction of peptides with membranes. Interaction of shock waves with biomembranes, cavitation effect and traumatic brain injury. Structure and dynamics of water and aqueous solutions at interfaces and in bulk, nature of the hydrophobic interactions, nature of the hydration force. Statistical mechanics of macromolecules, physics of soft matter.

Publications of Max L. Berkowitz

1. M. Berkowitz and K. M. Salikhov, Effect of Rotational Diffusion on the Exchange Broadening of EPR Spectra, Theoretical and Experimental Chemistry (English Translation) 9, 459-463 (1973).

2. V. Yakhot, M. Berkowitz and R. B. Gerber, Theory of Excimer Vibrational Relaxation and U. V. Emission in Solid Neon, Chem. Phys. 10, 61-66 (1975).

3. M. Berkowitz and R. B. Gerber, Vibrational Relaxation of Molecules in Solids: The Role of Rotational and of Translational Local Modes, Chem. Phys. Lett. 49, 260-264 (1977).

4. R. B. Gerber and M. Berkowitz, Role of Rotational and Translational Local Modes in Vibrational Relaxation in Solids: A Study of NH and ND in Solid Ar, Phys. Rev. Lett. 39, 1000-1004 (1977).

5. R. B. Gerber and M. Berkowitz, Rotational Mode Participation in Long-Distance Vibrational Energy Transfer in Solids, Chem. Phys. Lett. 56, 105-108 (1978).

6. R. B. Gerber, M. Berkowitz and V. Yakhot, Vibrational Relaxation of Molecular Impurities in Host Crystals, Mol. Phys. 36, 355--363 (1978).

7. M. Berkowitz and R. B. Gerber, Theory of Vibrational Relaxation in Solids: The Competition Between Local Phonon and Roton Receiving Modes, Chem. Phys. 37, 369-388 (1979).

8. M. Berkowitz, C. Brooks III and S. A. Adelman, Generalized Langevin Theory for Many-Body Problems in Chemical Dynamics: Modelling of Solid and Liquid State Response Functions, J. Chem. Phys. 72, 3889-3898 (1980).

9. M. Berkowitz and S. A. Adelman, Molecular Pair Effects and the Breakdown of Onsager's Dielectric Theory, J. Chem. Phys. 72, 4795-4798 (1980).

10. C. Brooks, III, M. Berkowitz and S. A. Adelman, Generalized Langevin Theory for Many-Body Problems in Chemical Dynamics: Gas-Surface Collisions, Vibrational Energy Relaxation in Solids, and Recombination Reactions in Liquids, J. Chem. Phys. 73, 4353-4364 (1980).

11. M. Berkowitz and J. A. McCammon, Brownian Motion of a System of Coupled Harmonic Oscillators, J. Chem. Phys. 75, 957-961 (1981).

12. M. Berkowitz, J. D. Morgan, D. J. Kouri and J. A. McCammon, Memory Kernels from Molecular Dynamics, J. Chem. Phys. 75, 2462-2463 (1981).

13. M. Berkowitz, D. J. Kouri and J. A. McCammon, Surface Temperature Effects in Molecule-Surface Collisions, J. Phys. Chem. 86, 2669-2671 (1982).

14. M. Berkowitz and J. A. McCammon, Molecular Dynamics with Stochastic Boundary Conditions, Chem. Phys. Lett. 90, 215-217 (1982).

15. M. Berkowitz, J. D. Morgan and J. A. McCammon, Generalized Langevin Dynamics Simulations with Arbitrary Time-Dependent Memory Kernels, J. Chem. Phys. 78, 3256-3261 (1983).

16. M. Berkowitz, J. D. Morgan, J. A. McCammon and S. H. Northrup, Diffusion-Controlled Reactions: A Variational Formula for the Optimum Reaction Coordinate, J. Chem. Phys. 79, 5563-5565 (1983).

17. M. Berkowitz, O. Karim, J. A. McCammon and P. Rossky, Sodium Chloride Ion Pair Interaction in Water: Computer Simulation, Chem. Phys. Lett. 105, 577-580 (1984).

18. S. K. Ghosh, M. Berkowitz and R. G. Parr, Transcription of Ground State Density-Functional Theory into a Local Thermodynamics, Proc. Natl. Acad. Sci. USA 81, 8028-8031 (1984).

19. A. C. Belch and M. Berkowitz, Molecular Dynamics Simulations of TIPS2 Water Restricted by a Spherical Hydrophobic Boundary, Chem. Phys. Lett. 113, 278-282 (1985).

20. S. K. Ghosh and M. Berkowitz, A Classical Fluid-Like Approach to the Density-Functional Formalism of Many Electron Systems, J. Chem. Phys. 83, 2976-2983 (1985).

21. M. Berkowitz, S. Ghosh and R. G. Parr, On the Concept of Local Hardness in Chemistry, J. Amer. Chem. Soc. 107, 6811-6814 (1985).

22. M. Berkowitz, Sodium Chloride Ion Pair Interaction in Water, in Molecular Dynamics and Protein Structure J. Hermans, Ed. Polycrystal Book Service, Western Springs, Illinois, pp. 35-36 (1985)

23. A. C. Belch, M. Berkowitz and J. A. McCammon, Solvation Structure of a Sodium Chloride Ion Pair in Water, J. Amer. Chem. Soc. 108, 1755-1761 (1986).

24. M. Berkowitz, Exponential Approximation for the Density Matrix and the Wigner Distribution, Chem. Phys. Lett. 129, 486-488 (1986).

25. M. Berkowitz and W. Wan, The Limiting Ionic Conductivity of Na^+ and Cl^- Ions in Aqueous Solutions. Molecular Dynamics Simulations, J. Chem. Phys. 86, 376-382 (1987).

26. M. Berkowitz, Density Functional Approach to Frontier Controlled Reactions, J. Am. Chem. Soc. 109, 4823-4825 (1987).

27. R. Reddy and M. Berkowitz, Structure and Dynamics of High-Pressure TIP4P Water, J. Chem. Phys. 87,6682-6686 (1987)

28. M. Berkowitz, R. G. Parr, Molecular Hardness and Softness, Local Hardness and Softness, Hardness and Softness, Hardness and Softness Kernels, and Relations Among These Quantities, J. Chem. Phys 88, 2554 (1988).

29. R. Reddy and M. Berkowitz, Temperature Dependence of Conductance of the Li^+ , Cs^+ and Cl^- Ions in Water: Molecular Dynamics Simulation, J. Chem. Phys. 88, 7104-7110 (1988).

30. M. R. Reddy and M. Berkowitz, Conductance of Cs^+ Ion in Water: Molecular Dynamics Simulation, J. Solut. Chem. 17, 1183-1191 (1988).

31. M. R. Reddy and M. Berkowitz, Dielectric Constant of SPCE Water, Chem. Phys. Lett. 155, 173-176 (1989).

32. M. R. Reddy and M. Berkowitz, Hydration Forces Between Parallel DNA Double Helices: Computer Simulations, Proc. Natl. Acad. Sciences, 86, 3165 (1989).

33. M. R. Reddy, K. Foster and M. Berkowitz, Structure and Dynamics of Water Between Segments of Parallel DNA Molecules, J. Mol. Liq., 41, 181-192 (1989).

34. K. Foster, K. Raghavan and M. Berkowitz, A Molecular Dynamics Study of the Effect of Temperature on the Structure and Dynamics of Water Between Pt Walls, Chem. Phys. Lett. 162, 32 (1989).

35. K. Motakabbir and M. Berkowitz, Isothermal Compressibility of SPCE Water, J. Phys. Chem. 94, 8359 (1990)

36. K. Motakabbir and M. Berkowitz, Liquid-Vapor Interface of TIP4P Water: Comparison Between a Polarizable and a Non-polarizable Model, Chem. Phys. Lett. 176, 61 (1991)

37. K. Raghavan, K. Foster, K. Motakabbir and M. Berkowitz, Structure and Dynamics of Water at the Pt(111) Interface: Molecular Dynamics Study, J. Chem. Phys. 94, 2110 (1991)

38. K. Raghavan, K. Foster, and M. Berkowitz, Comparison of the Structure and Dynamics of Water at the Pt(111) and Pt(100) Interfaces: Molecular Dynamics Study, Chem. Phys. Lett. 177, 426 (1991)

39. M. Berkowitz and K. Raghavan, Computer Simulation of the Membrane/Water Interface, Langmuir 7, 1042 (1991)

40. L. Perera and M. Berkowitz, Many-Body Effects in Molecular Dynamics Simulations of $Na^+(H_2O)_n$ and $Cl^-(H_2O)_n$ Clusters, J. Chem. Phys. 95, 1954 (1991)

41. K. Raghavan. M. Rami Reddy and M. Berkowitz, A Molecular Dynamics Study of the Structure and Dynamics of Water Between DLPE Bilayers, Langmuir 8, 233 (1992).

42. L. Perera and M. Berkowitz, Dynamics of Ionic Solvation in Stockmayer Fluid, J. Chem. Phys. 96, 3092 (1992).

43. L. Perera and M. Berkowitz, Structure and Dynamics of $Cl^-(H_2O)_{20}$ Clusters. The Effect of the Polarizability and the Charge of the Ion, J. Chem. Phys. 96, 8288 (1992)

44. I. I. Vaisman and M. Berkowitz, Local Structural Order and Molecular Associations in Water-DMSO Mixtures. Molecular Dynamics Study, J. of Amer. Chem. Soc. 114, 7889 (1992)

45. L. Perera and M. Berkowitz, Ultra-fast Solvation Dynamics in a Stockmayer Fluid, J. Chem. Phys. 97, 5253 (1992).

46. I. Vaisman, L. Perera and M. Berkowitz, Mobility of Stretched Water, J. Chem. Phys. 98, 9859 (1993)

47. L. Perera and M. Berkowitz, Stabilization Energies of Chloride Ion in Water Clusters, J. Chem. Phys. 99, (1993)

48. L. Perera and M. Berkowitz, Solvation Dynamics in Stockmayer Fluids, in Condensed Matter Theories, Vol. 8, Edited by L. Blum and F. Malik, Plenum Press, New York, 1993.

49. L. Perera and M. Berkowitz, Ion Solvation in Water Clusters, Z. fur Physik D, 26, 166 (1993)

50. S. J. Marrink, M. Berkowitz and H.J.C. Berendsen, Molecular Dynamics Simulations of a Water/Membrane Interface: the Ordering of Water and its Relation to the Hydration Force, Langmuir 9, 3122 (1993).

51. L. Perera and M. Berkowitz, Free Energy Profiles for Li^+ and F^- Ions Approaching Pt(100) Surface: Molecular Dynamics Study, J. Phys. Chem. 97, 13803 (1993).

52. L. Perera and M. Berkowitz, Structures of $Cl^-(H_2O)_n$ and $F^-(H_2O)_n$ (n=2,3,...15) clusters. Molecular Dynamics Computer Simulations, J. Chem. Phys. 100, 3085 (1994).

53. L.S. Sremaniak, L. Perera and M. Berkowitz, Enthalpies of Formation and Stabilization Energies of $Br^-(H_2O)_n$ (n=1,2,...15) clusters. Comparison between Molecular Dynamics Computer Simulations and Experiment, Chem. Phys. Lett. 218, 377 (1994).

54. M. Berkowitz and K. Raghavan, Electrostatics of a Water/Membrane Interface, chapter in *Biomembrane Electrochemistry*, M. Blanck and I Vodyanoy editors, ACS advances in chemistry series, vol 235 , (ACS, Washington DC., 1994).

55. X. Xia and M. Berkowitz, Effect of Ion-Electrode Contact on the Energetics of the Heterogeneous Electron Transfer, Chem. Phys. Lett. 227, 561 (1994)

56. L. Perera and M. Berkowitz, Molecular Dynamics Computer Simulations of Aqueous Solution/Platinum Interface, Chapter in *Theoretical and Computational Approaches to Interface Phenomena*" H. Sellers and J. Golab ed. (Plenum, New York, 1994)

57. L. Perera, U. Essmann and M. Berkowitz, The Effect of the Treatment of Long Range Forces on the Dynamics of Ions in Aqueous Solutions, J. Chem. Phys. 102, 450 (1995)

58. S.J. Marrink and M. Berkowitz, Water and Membranes, Chapter in *Permeability and Stability of Lipid Bilayers*, A. Disalvo and S. Simon editors, (CRC Press 1995).

59. X.Xia and M. Berkowitz, The Electric Field Induced Restructuring of Water at Platinum/Water Interface. Molecular Dynamics Computer Simulation, Phys. Rev. Lett. 74, 3193 (1995)

60. X. Xia, L. Perera, U. Essmann and M. Berkowitz, The Structure of Water at Pt/Water Interface. Molecular Dynamics Computer Simulations, Surf. Science 335, 401 (1995).

61. U. Essmann, L. Perera and M. Berkowitz, The origin of the Hydration Interaction of Lipid Bilayers from MD Simulation of DPPC Membranes in Gel and Liquid Crystalline Phase, Langmuir 11, 4519 (1995).

62. U. Essmann, L. Perera and M. Berkowitz, T. Darden, H. Lee and L. G. Pedersen, A Smooth Particle Ewald Method, J. Chem. Phys. 103, 8577 (1995)

63. L. Sremaniak, L. Perera and M. Berkowitz, Thermally Induced Structural Changes in $F^-(H_2O)_{11}$ and $Cl^-(H_2O)_{11}$ clusters: Molecular Dynamics Computer Simulations, J. Phys. Chem. 100, 1350, (1996).

64. L. Perera, U. Essmann and M. Berkowitz, The Role of Water in the Hydration Force Acting between Lipid Bilayers, Langmuir 12, 2625 (1996)

65. K. J. Schweighofer, X. Xia and M. Berkowitz, A Molecular Dynamics Study of Water next to Electrified Ag(111) Surfaces, Langmuir 12, 3747-3752 (1996)

66. G. Markovich, L. Perera, M. Berkowitz and O. Cheshnovsky, The Solvation of Cl^-, Br^- and I^- in Acetonitrile Clusters: Photoelectron Spectroscopy and Molecular Dynamics Simulations, J. Chem. Phys. 105, 2675-2685 (1996).

67. L. Sremaniak, L. Perera and M. Berkowitz, Cube to Cage Transitions in $(H_2O)_n$ (n=12,16 and 20), J. Chem. Phys. 105, 3715-3721(1996).

68. I.C. Yeh, L. Perera and M. Berkowitz, Photodetachment Spectra of $Cl^-(H_2O)_n$ clusters. Predictions and Comparisons. Chem. Phys. Lett. 264, 31-38 (1997)

69. K.J. Schweighofer, U. Essmann and M. Berkowitz, Simulation of Sodium Dodecyl Sulfate (SDS) at the Water-Carbon Tetrachloride Interfaces at Low Surface Coverage. J. Phys. Chem. 101, 3793-3799 (1997).

70. L. Perera, U. Essmann and M. Berkowitz, The Role of Water in the Hydration Force. Molecular Dynamics Computer Simulations. Progress in Colloid and Polymer Science 103, 107-115 (1997).

71. P. Itskowitz and M. Berkowitz, Chemical Potential Equilization Principle: Direct Approach from Density Functional Theory, J. Phys. Chem. 101, 5687-5691 (1997).

72. K.J. Schweighofer, U. Essmann and M. Berkowitz, Structure and Dynamics of Water in the Presence of Charged Surfactant Monolayers at the Water-CCl_4 Interface. A Molecular Dynamics Study J. Phys. Chem. 101 10775-10780 (1997).

73. P. Itskowitz and M. Berkowitz, Molecular and Atomic Dipole Moments in Heteronuclear and Homonuclear Diatomics. Density Functional Approach. J. Phys. Chem. A. 102, 4808-4812 (1998).

74. I.C. Yeh and M. Berkowitz, Structure and Dynamics of Water at Water/Pt Interface as Seen by Molecular Dynamics Computer Simulations. J. Electroanalytical Chem. 450 (1998).

75. P. Itskowitz and M. Berkowitz, Molecular Polarizability and Atomic Properties. Density Functional Approach. J. Chem. Phys. 109, 10142 (1998)

76. A. Smondyrev and M.L. Berkowitz, Molecular Dynamics Study of Sn-1 and Sn-2 Chain Conformations in DPPC Membranes, J. Chem. Phys. 110, 3981-3985 (1999).

77. U. Essmann and M.L. Berkowitz, Dynamical Properties of Phospholipid Bilayers from Computer Simulation, Biophys. J 76, 2081-2089 (1999)

78. I.C. Yeh and M. Berkowitz, Aqueous Solutions near Charged Ag(111) Surface: Comparison between a Computer Simulation and Experiment, Chem. Phys. Lett., 301, 81-86 (1999).

79. A. Smondyrev and M.L. Berkowitz, United Atom Force Field for Phospholipid Membranes. Constant Pressure Molecular Dynamics Simulation of DPPC/Water System. J. Comp. Chem. 20, 531-545 (1999)

80. M. L. Berkowitz, I.C. Yeh and E. Spohr, Structure of Water at Water/Metal Interface. Molecular Dynamics Computer Simulations, Chapter in "Interfacial Electrochemistry" CRC Press, A. Wieckowski ed. (1999).

81. I.C. Yeh and M. Berkowitz, Dielectric Constant of Water at High Electric Field: Molecular Dynamics Study, J. Chem. Phys. 110, 7935-7942 (1999)

82. A. Smondyrev and M.L. Berkowitz, Molecular Dynamics Simulation of DPPC Bilayer in DMSO, Biophys. J 76, 2472-2478 (1999)

83. I.C. Yeh and M. Berkowitz, Ewald Summation for Systems with Slab Geometry, J. Chem. Phys. 111, 3155-3162 (1999)

84. A. Smondyrev and M.L. Berkowitz, Structure of DPPC/Cholesterol Bilayer at Low and High Cholesterol Concentrations: Molecular Dynamics Simulations, Biophys. J 77, 2075-2089 (1999).

85. H. Dominguez, A.M. Smondyrev and M.L. Berkowitz, Computer Simulation of Phosphatidylcholine Monolayers at Air/Water and Carbontetrachloride/Water Interfaces, J. Phys. Chem. B 103, 9582-9588 (1999).

86. A. Smondyrev and M. Berkowitz, Molecular dynamics simulation of fluorination effects on phospholipid bilayer , J. Chem. Phys. 111, 9864-9870 (1999).

87. A. M. Smondyrev and M.L. Berkowitz, Molecular Dynamics Simulation of DPPC Membrane with Cholesterol Sulfate, Biophys. J. 78, 1672-1680 (2000).

88. H. Dominguez and M.L. Berkowitz, Computer Simulations of Sodium Dodecyl Sulfate at Liquid/Liquid and Liquid/Vapor Interfaces, J. Phys. Chem. B. 104,5302-5308 (2000).

89. IC Yeh and M.L. Berkowitz, Effects of the Polarizability and Water Density Constraint on the Structure of Water Near Charged Surfaces: Molecular Dynamics Simulations, J. Chem. Phys.,112, 10491-10495 (2000)

90. A. M. Smondyrev and M.L. Berkowitz, Molecular Dynamics Simulation of the Structure of Dimyristoylphosphatidylcholine Bilayers with Cholesterol, Ergosterol, and Lanosterol, Biophys J, 80, 1649-1658 (2001)

91. A. M. Smondyrev and M.L. Berkowitz, Effect of oxygenated sterol on phospholipid bilayer properties: a molecular dynamics simulation, Chem. Phys. Lipids 112, 31-39 (2001)

92. S. Senapati and M.L. Berkowitz, Computer simulation study of the interface width of the liquid/liquid interface, Phys. Rev. Lett. 87, 176101 (2001)

93. S. A. Pandit and M. L. Berkowitz, Molecular Dynamics Simulation of Dipalmitoylphosphatidylserine Bilayer with Na^+ counterions, Biophysical Journal, **82** 1818–1827 (2002)

94. C.D. Bruce, M.L. Berkowitz, L.Perera , M.D.E. Forbes, Molecular dynamics simulation of sodium dodecyl sulfate micelle in water: Micellar structural characteristics and counterion distribution, J. Phys. Chem. B. 106, 3788-3793 (2002)

95. C.D. Bruce, S. Senapati, M.L. Berkowitz, L.Perera , M.D.E. Forbes, Molecular dynamics simulation of sodium dodecyl sulfate micelle in water: The behavior of water, J. Phys. Chem. B. 106, 10902-10907 (2002)

96. S. Senapati, J.S. Keiper, J.M. DeSimone, G. D. Wignall, Y. B. Melnichenko, H. Frielinghaus and M.L. Berkowitz, Structure of phosphate fluorosurfactant based reverse micelles in supercritical carbon dioxide, Langmuir, 18 7371-7376 (2002)

97. S. Senapati and M.L. Berkowitz, Water structure and dynamics in phosphate fluorosurfactant based reverse micelle: Molecular dynamics simulation, J. Chem. Phys. 118, 1937 – 1944 (2003).

98. I. M. Withers, A. V. Dobrynin, M.L. Berkowitz, and M. Rubinstein. Monte Carlo simulation of homopolymer chains. I. Second virial coefficient. J. Chem. Phys. 118, 4721-4732 (2003).

99. S. Pandit, D. Bostick and M.L. Berkowitz, Molecular dynamics simulation of dipalmitoylphosphatidylcholine bilayer with NaCl, Biophys. J. 84, 3743-3750 (2003).

100. D. Bostick and M.L. Berkowitz, The implementation of slab geometry for membrane-channel molecular dynamics simulations, Biophys. J. 85, 97-107 (2003)

101. S. Pandit, D. Bostick and M.L. Berkowitz, An algorithm to describe molecular scale rugged surfaces and its application to a study of water/lipid bilayer interface, J. Chem. Phys. 119, 2199-2205 (2003).

102. S. Pandit, D. Bostick and M.L. Berkowitz, Mixed Bilayer Containing Dipalmitoylphosphatidylcholine and Dipalmitoylphosphatidylserine: Lipid Complexation, Ion Binding, and Electrostatics, Biophys. J. 85, 3120-3131 (2003).

103. S. Senapati and M. L. Berkowitz, Molecular Dynamics Simulation Studies of Polyether and Perfluoropolyether Surfactant Based Reverse Micelles in Supercritical Carbon Dioxide J. Phys. Chem. B. 107, 12906-12916 (2003).

104. S. Pandit, D. Bostick and M.L. Berkowitz, Complexation of Phosphatidylcholine Lipids with Cholesterol, Biophys. J. 86, 1345-1356 (2004).

105**.** L. Lu and M. L. Berkowitz, Molecular Dynamics Simulation of a Reverse Micelle Self Assembly in Supercritical CO_2. J. Am. Chem. Soc. 126, 10254-10255, (2004).

106. S. Senapati and M. L. Berkowitz, Computer Simulation Studies of Water States in Perfluoro Polyether Reverse Micelles: Effects of Changing the Counterion. J. Phys. Chem. A. 108, 9768-9776, (2004).

107. D. L. Bostick and M. L. Berkowitz, Exterior Site Occupancy Infers Chloride-Induced Proton Gating in a Prokaryotic Homolog of the ClC Chloride Channel. Biophys. J. 87, 1686-1696, (2004)

108. S. Y. Bhide and M. L. Berkowitz , Structure and Dynamics of Water at The Interface with Phospholipid Bilayers. J. Chem. Phys. 123 (22): Art. No. 224702 (2005).

109. L. Lu and M. L. Berkowitz, The Effect of the Rigidity of Perfluoropolyether Surfactant on its Behavior at the Water/Supercritical Carbon Dioxide Interface. J. Phys. Chem. B, 109, 21725-21731 (2005)

110. M. L. Berkowitz, D. L. Bostick, and S. Pandit, Aqueous Solutions next to Phospholipid Membrane Surfaces: Insights from Simulations. Chem. Rev. 106 1527-1539 (2006)

111. L. Lu and M.L. Berkowitz, Hydration force between model hydrophilic surfaces: Computer simulations. J. Chem. Phys. 124, Art. No. 101101 (2006).

112. Shreyas Y. Bhide and Max L. Berkowitz, The behavior of reorientational correlation functions of water at the water/lipid bilayer interface, J. Chem. Phys. 125,094713 (2006)

113. L. Lu and M.L. Berkowitz, The effect of water structure and surface charge correlations on the hydration force acting between model hydrophilic surfaces. Mol. Physics. 104 3607 (2006)

114. S. Y. Bhide, Z. Zhang and M. L. Berkowitz, Molecular Dynamics Simulations of SOPS and Sphingomyelin Bilayers Containing Cholesterol , Biophys. J. 92, 1284-1295 (2007)

115. Z. Zhang, S. Bhide and M.L. Berkowitz, "Molecular Dynamics Simulations of Bilayers Containing Mixtures of Sphingomyelin with Cholesterol and Phosphatidylcholine with Cholesterol", J. Phys. Chem. B, **111,** 12888-12897 (2007).

116. M. Berkowitz, On the Nature of Lipid Rafts: Insights from the Molecular Detailed Simulations of Model Biological Membranes containing Mixtures of Cholesterol and Phospholipids. Chapter in a book on membranes In book series: "Current topics in membranes" vol. 60, 257-279 (2008).

117. Z. Zhang, L.Lu and M.L. Berkowitz, "Energetics of cholesterol transfer between lipid bilayers", J. Phys. Chem. B, 112, 3807-3811 (2008)

118. R. Vacha, D. Horinek, M.L. Berkowitz and P. Jungwirth, Hydronium and hydroxide at the interface between water and hydrophobic media**.** Phys Chem. Chem. Phys. 10, 4975-4980 **(**2008)

119. M. L. Berkowitz, Detailed Molecular Dynamics Simulations of Model Biological Membranes Containing Cholesterol. Bioph. Bioch. Acta, 1788 86-96 (2009).

120. C. H. Davis and M.L. Berkowitz, Interaction between Amyloid-beta (1-42) peptide and Phospholipid Bilayer: A Molecular Dynamics Study Biophys. J 96, 785-796 (2009).

121 Robert Vácha, Max L. Berkowitz, and Pavel Jungwirth, Molecular Model of a Cell Plasma Membrane with an Asymmetric Multicomponent Composition: Water Permeation and Ion Effects, Biophys. J. 96, 4493 - 4501 (2009)

122. Zhancheng Zhang and Max L. Berkowitz, Orientational Dynamics of Water in Phospholipid Bilayers with Different Hydration Levels, J. Phys. Chem. B 113, 7676-7680 (2009)

123 Robert Vácha, Shirley W. I. Siu, Michal Petrov, Rainer A. Böckmann, Justyna Barucha-Kraszewska, Piotr Jurkiewicz, Martin Hof, Max L. Berkowitz and Pavel Jungwirth Effects of alkali cations and halide anions on the DOPC lipid membrane, J. Phys. Chem. A 113, 7235-7243 (2009)

124. C. Eun and M. L. Berkowitz, Origin of the hydration force: Water-mediated interaction between two hydrophilic plates, J. Phys. Chem. B 113, 13222-13228 (2009).

125. C.H. Davis and M.L. Berkowitz, Structure of the Amyloid-beta (1-42) Monomer Absorbed To Model Phospholipid Bilayers: A Molecular Dynamics Study, J. Phys. Chem. B 113, 14480-14486 (2009)

126. C. Eun and M.L. Berkowitz, Thermodynamic and Hydrogen Bonding Analyses of the Interaction between Model Lipid Bilayers, J. Phys. Chem. B. 114, 3013-3019 (2010)

127.R. Vacha, P. Jurkiewicz; M. Petrov ; M. L. Berkowitz; R.A. Bockmann; J. Barucha-Kraszewska ; M. Hof, M ; P. Jungwirth. Mechanism of Interaction of Monovalent Ions with Phosphatidylcholine Lipid Membranes , J. Phys. Chem. , 114 (29): 9504-9509 (2010)

128. C.H. Davis; M.L. Berkowitz. A molecular dynamics study of the early stages of amyloid-beta(1-42) oligomerization: The role of lipid membranes Proteins-Structure Function and Bioinformatics 78 (11): 2533-2545 (2010)

129. C. Eun; M.L. Berkowitz. Fluctuations in Number of Water Molecules Confined between Nanoparticles, J. Phys. Chem. B, 114 (42): 13410-13414 (2010)

130. M.L. Berkowitz and J. T. Kindt, Molecular Detailed Simulations of Lipid Bilayers, Chapter in Reviews in Computational Chemistry, Vol. 27, Wiley, (2011)

131. C. Eun; M.L. Berkowitz, Molecular Dynamics Simulation Study of Interaction between Model Rough Hydrophobic Surfaces, J. Phys. Chem. A, 115 6059-6067 (2011)

132. M. Watkins, M. L. Berkowitz and A. L. Shluger; Role of water in atomic resolution AFM in solutions. PCCP, 13, 12584-12594 (2011)

133. J. Das, C. Eun, S. Perkin, and M. L. Berkowitz; Restructuring of Hydrophobic Surfaces Created by Surfactant Adsorption to Mica Surfaces, Langmuir, 27, 11737-11741 (2011)

134. S. J. Irudayam and M.L. Berkowitz; Influence of the arrangement and secondary structure of melittin peptides on the formation and stability of toroidal pores, Biochimica Et Biophysica Acta-Biomembranes, 1808, 2258-2266 (2011)

135. M.L. Berkowitz and R. Vacha, Aqueous Solutions at the Interface with Phospholipid Bilayers, Accounts of Chemical Research, 45, 74-82 (2012)

136. C.Eun and M.L.Berkowitz, Molecular dynamics simulation study of the water-mediated interaction between zwitterionic and charged surfaces, Journal of Chemical Physics, 136, 024501 (2012)

137. K. Santo and M.L.Berkowitz, Difference between Magainin-2 and Melittin Assemblies in Phosphatidylcholine Bilayers: Results from Coarse-Grained Simulations, Journal Of Physical Chemistry B, 116 3021-3030 (2012)

138. N. Gosvami, E. Parsons, C. Markovich, M.L. Berkowitz, B.W. Hoogenboom and S. Perkin, Resolving the structure of a model hydrophobic surface: DODAB monolayers on mica, RSC Advances, 2, 4181-4188 (2012)

139. S. J. Irudayam and M.L. Berkowitz; Binding and reorientation of melittin in POPC bilayer: Computer simulations, Biochimica Et Biophysica Acta-Biomembranes, 1818, 2975-2981 (2012)

140. K. P. Santo, S.J. Irudayam and M.L. Berkowitz, Melittin creates transient pores in a lipid bilayer; Results from computer simulations, Journal of Physical Chemistry B, 117, 5031-5042 (2013)

141. S.J. Irudayam, T. Pobandt and M. L. Berkowitz, Free Energy Barrier for Melittin Reorientation from a Membrane-Bound State to a Transmembrane State, Journal Of Physical Chemistry B, 117, 13457-13463 (2013)

142. C. Eun, J. Das and M. L. Berkowitz, Restructuring of a Model Hydrophobic Surface: Monte Carlo Simulations Using a Simple Coarse-Grained Model, Journal Of Physical Chemistry B, 117, 15584-15590 (2013)

143. K.P. Santo and M.L. Berkowitz, Shock wave interaction with a phospholipid membrane: coarse-grained computer simulations, Journal of Chemical Physics, 140, 054906 (2014)

144. A. Goliaei, K. P. Santo, M.L. Berkowitz, Local Pressure Changes in Lipid Bilayers Due to Adsorption of Melittin and Magainin-h2 Antimicrobial Peptides: Results from Computer Simulations, Journal of Phys. Chemistry B, 118, 12673-12679 (2014)

145. Y. Yao, Y. Kanai, M.L. Berkowitz, Role of Charge Transfer in Water Diffusivity in Aqueous Ionic Solutions, Journal of Physical Chemistry Letters, 5, 2711-2716 (2014)

146. K. P. Santo and M. L. Berkowitz, Shock Wave Induced Collapse of Arrays of Nanobubbles Located Next to a Lipid Membrane: Coarse-Grained Computer Simulations. Journal of Physical Chemistry B, *119*, 8879–8889 **(**2015)

147. U. Adhikari, A. Goliaei and M. L. Berkowitz, Mechanism of Membrane Poration by Shock Wave Induced Nanobubble Collapse: A Molecular Dynamics Study. Journal of Physical Chemistry B, 119, 6225-6234 (2015)

148. A. Goliaei, U. Adhikari and M.L. Berkowitz, Opening of the Blood-Brain Barrier Tight Junction Due to Shock Wave Induced Bubble Collapse: A Molecular Dynamics Simulation Study, ACS Chem. Neuroscience 6, 1296-1301 (2015)

149 Y. Yao, M. L. Berkowitz, and Yosuke Kanai, Modeling of concentration dependent water diffusivity in ionic solutions: Role of intermolecular charge transfer, J. of Chemical Physics 143, 241101 (2015)

150 M. Berkowitz A Molecular Look at membranes, Chapter in a book Current Topic in Membranes Academic Press publisher, 77, 1-25 (2016)

151 E. Y. Lau, M. L. Berkowitz, and E. Schwegler, Shock Wave-Induced Damage of a Protein by Void Collapse, Biophysical Journal 110, 147–156 (2016)

152. A. Upendra, A. Goliaei, L. Tsereteli and M. L. Berkowitz, Properties of Poloxamer Molecules and Poloxamer Micelles Dissolved in Water and Next to Lipid Bilayers: Results from Computer Simulations; J. of Phys. Chem. B. 120, 5823-5830 (2016)

153. A. Goliaei, E. Lau, U. Adhikari, E. Schwegler and M.L. Berkowitz, Behavior of P85 and P188 Poloxamer Molecules: Computer Simulations Using United-Atom Force-Field, J. Phys. Chem. B. 120, 8631-8641 (2016).