ATHANASSIOS Z. PANAGIOTOPOULOS

EDUCATION

Dipl. Eng. (5-year degree) in Chemical Engineering,
National Technical University of Athens, Greece (1982)

Ph.D.,
Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA (1986)

Postdoctoral,
Physical Chemistry Laboratory, University of Oxford, United Kingdom (1986-1987)

PROFESSIONAL POSITIONS

School of Chemical Engineering, Cornell University, Ithaca, NY
Assistant Professor (1987-92), Assoc. Professor (1992-97), Professor (1998-99, on leave)

Democritus National Research Center, Athens, Greece, Visiting Scientist (1993-94, 2020)

Institute for Physical Science and Technology and Department of Chemical Engineering, University of Maryland, College Park, MD, Professor (1997-2000)

Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ
Professor (2000-2006), Director of Graduate Studies (2003-05, 2013-14), Susan Dod Brown Professor (2007-present), Department Chair (2016-2022)

SELECTED HONORS

AIChE AXΣ Award for Chemical Engineering Research, 2024
BASF Lectureship, Wayne State U., 2021
SEAS Distinguished Teacher Award, Princeton U., 2020
Robert L. Pigford Memorial Lecturer, U. of Delaware, 2018
Keith E. Gubbins Inaugural Lecturer, N. Carolina State U., 2016
Chemical Engineering Distinguished Lecturer, Texas A&M at Qatar, 2013
Elected to the American Academy of Arts and Sciences, 2012
Elected to the National Academy of Engineering, 2004
J.M. Prausnitz Award for Achievement in Applied Chemical Thermodynamics, 1998
Colburn Award of the American Institute of Chemical Engineers, 1995

PROFESSIONAL AFFILIATIONS

American Institute of Chemical Engineers (elected Fellow in 2014)
American Chemical Society
American Physical Society
American Association for the Advancement of Science (elected Fellow in 2012)

EDITORIAL, ADVISORY BOARD, AND COUNCIL MEMBERSHIPS

J. Chem. Phys., Editorial Advisory Board, 2020 – 2022
Molecular Physics, Advisory Board, 2008 – 2023; Editorial Board, 2023 – present
AIChE J., Contributing Editors Board, 2012 – 2020
Midwest Integrated Center for Computational Materials Sci. Advisory Board, 2017 – present

BOOK

Essential Thermodynamics, Drios Press, 2011 (undergraduate textbook)

REFEREED PUBLICATIONS

Citation data as of Sept. 20, 2024: Google Scholar: 27,258 total citations, h=82; Web of Science: 22,427 total citations, h=74.

1. A. Z. Panagiotopoulos and S. K. Kumar, "A generalized technique to obtain pure component parameters for two-parameter equations of state," *Fluid Phase Equilibria*, **22**: 77-88 (1985). DOI: 10.1016/0378-3812(85)87012-6 *[Web of Science citations: 22]*
2. A. Z. Panagiotopoulos and R. C. Reid, "New mixing rule for cubic equations of state for highly polar, asymmetric systems," *ACS Symposium Ser.*, **300**: 571-582 (1986). DOI: 10.1021/bk-1986-0300.ch028 *[211]*
3. A. Z. Panagiotopoulos and R. C. Reid, "Multiphase high-pressure equilibria in ternary aqueous systems," *Fluid Phase Equilibria*, **29**: 525-534 (1986). DOI: 10.1016/0378-3812(86)85051-8 *[79]*
4. A. Z. Panagiotopoulos and R. C. Reid, "On the relationship between pair-wise fluctuations and thermodynamic derivatives," *J. Chem. Phys.*, **85**: 4650-4653 (1986). DOI: 10.1063/1.451761 *[19]*
5. A. Z. Panagiotopoulos, U. W. Suter, and R. C. Reid, "Phase diagrams of non-ideal fluid mixtures from Monte-Carlo simulation," *Ind. Eng. Chem. Fundam.*, **25**: 525-535 (1986). DOI: 10.1021/i100024a012 *[70]*
6. A. Z. Panagiotopoulos and R. C. Reid, "High pressure phase equilibria in ternary mixtures with a supercritical component," *ACS Symposium Ser.*, **329**: 115-129 (1987). DOI: 10.1021/bk-1987-0329.ch010 *[32]*
7. A. Z. Panagiotopoulos, "Direct determination of phase coexistence properties of fluids by Monte Carlo simulation in a new ensemble," *Mol. Phys.*, **61**: 813-826 (1987). Reprinted in the special issue "Defining Papers in Molecular Physics, 1958-2001" **100**: 237-46 (2002). DOI: 10.1080/00268978700101491 *[1,922+28]*
8. A. Z. Panagiotopoulos, "Adsorption and capillary condensation of fluids in cylindrical pores by Monte Carlo simulation in the Gibbs ensemble," *Mol. Phys.*, **62**: 701-719 (1987). DOI: 10.1080/00268978700102501 *[290]*
9. G. B. Woods, A. Z. Panagiotopoulos, and J. S. Rowlinson, "Adsorption of fluids in model zeolite cavities," *Mol. Phys.*, **63**: 49-63 (1988). DOI: 10.1080/00268978800100051 *[124]*
10. A. Z. Panagiotopoulos, N. Quirke, M. Stapleton, and D. J. Tildesley, "Phase equilibria by simulation in the Gibbs ensemble: alternative derivation, generalization and application to mixture and membrane equilibria," *Mol. Phys.*, **63**: 527-545 (1988). DOI: 10.1080/00268978800100361 *[1,124]*
11. A. Z. Panagiotopoulos, R. C. Wilson, and R. C. Reid, "Phase equilibria in ternary systems with carbon dioxide, water and carboxylic acids at elevated pressures," *J. Chem. Eng. Data*, **33**: 321-327 (1988). DOI: 10.1021/je00053a028 *[27]*
12. M. R. Stapleton, D. J. Tildesley, N. Quirke, and A. Z. Panagiotopoulos, "Phase equilibria of quadrupolar fluids by simulation in the Gibbs ensemble," *Mol. Simulation*, **2**: 147-162 (1989). DOI: 10.1080/08927028908031364 *[54]*

13. A. Z. Panagiotopoulos, "Exact calculations of fluid-phase equilibria by Monte Carlo simulation in a new statistical ensemble," *Int. J. Thermophys.* **10**: 447-457 (1989). DOI: 10.1007/BF01133541 *[115]*

14. A. Z. Panagiotopoulos, "Gibbs-ensemble Monte Carlo simulations of phase equilibria in supercritical fluid systems," *ACS Symposium Ser.*, **406**: 39-51 (1989). DOI: 10.1021/bk-1989-0406.ch004 *[12]*

15. A. Z. Panagiotopoulos and M. R. Stapleton, "The Gibbs method for calculating phase equilibria by simulation," *Fluid Phase Equilibria*, **53**: 133-141 (1989). DOI: 10.1016/0378-3812 (89)80080-9 *[40]*

16. K. E. Gubbins and A. Z. Panagiotopoulos, "Molecular Simulation," *Chem. Eng. Progress*, **85** (10): 23-27 (1989).

17. M. R. Stapleton and A. Z. Panagiotopoulos, "Application of excluded volume map sampling to phase equilibrium calculations in the Gibbs ensemble," *J. Chem. Phys.*, **92**: 1285-93 (1990). DOI: 10.1063/1.458138 *[65]*

18. R. C. Willson, A. Z. Panagiotopoulos, and R. C. Reid, "High-pressure phase equilibria in ternary systems of propionic acid and water with ethane, SF_6, or refrigerant 13 ($CClF_3$), 23 (CF_3H) or 116 (C_2F_6)," *J. Chem. Eng. Data,* **36**: 290-293 (1991). *[2]*

19. V. I. Harismiadis, K. K. Koutras, D. P. Tassios, and A. Z. Panagiotopoulos, "How good is conformal solutions theory for phase equilibrium predictions?" *Fluid Phase Equil.*, **65**: 1-18 (1991). DOI: 10.1016/0378-3812(91)87014-Z *[87]*

20. M. E. van Leeuwen, C. J. Peters, J. de Swaan Arons, and A. Z. Panagiotopoulos, "Evaluation of a statistical-mechanical virial equation of state using Gibbs-ensemble molecular simulation," *Fluid Phase Equilibria*, **66**: 41-55 (1991). DOI: 10.1016/..5046-W *[8]*

21. M. E. van Leeuwen, C. J. Peters, J. de Swaan Arons, and A. Z. Panagiotopoulos, "Investigation of the transition to liquid-liquid immiscibility for Lennard-Jones (12,6) systems using Gibbs-ensemble molecular simulations," *Fluid Phase Equilibria*, **66**: 57-75 (1991). DOI: 10.1016/0378-3812(91)85047-X *[32]*

22. S. K. Kumar, I. Szleifer, and A. Z. Panagiotopoulos, "Determination of chemical potentials in polymeric systems from Monte Carlo simulations," *Phys. Rev. Lett.*, **66**: 2935-2938 (1991). DOI: 10.1103/PhysRevLett.66.2935 *[163]*

23. A. Z. Panagiotopoulos, "Molecular simulation of fluid-phase equilibria: simple, ionic and polymeric fluids," *Fluid Phase Equil.*, **76**: 97-112 (1992); erratum in **92**, 313 (1994). DOI: 10.1016/0378-3812(92)85080-R *[139]*

24. A. Z. Panagiotopoulos, "Direct determination of fluid phase equilibria by simulation in the Gibbs ensemble: a review," *Mol. Simulation*, **9**: 1-23 (1992). DOI: 10.1080/08...48258 *[346]*

25. I. Szleifer, E. M. O' Toole, and A. Z. Panagiotopoulos, "Monte Carlo simulation of the collapse-coil transition in homopolymers," *J. Chem. Phys.*, **97**: 6802-8 (1992). DOI: 10.1063/1.463633 *[54]*

26. I. Szleifer and A. Z. Panagiotopoulos, "Chain length and density dependence of the chemical potential of lattice polymers," *J. Chem. Phys.*, **97**: 6666-73 (1992). DOI: 10.1063/1.463671 *[22]*

27. E. M. O' Toole and A. Z. Panagiotopoulos, "Monte Carlo simulation of folding transitions of simple model proteins using a chain growth algorithm," *J. Chem. Phys.*, **97**: 8644-52 (1992). DOI: 10.1063/1.463383 *[67]*

28. A. D. Mackie, E. M. O' Toole, D. A. Hammer, and A. Z. Panagiotopoulos, "Molecular simulation of self-assembly in surfactant and protein solutions," *Fluid Phase Equil.*, **82**: 251-260 (1993). DOI: 10.1016/0378-3812(93)87149-U *[11]*
29. G. Orkoulas and A. Z. Panagiotopoulos, "Chemical potentials in ionic systems from Monte Carlo simulations with distance-biased test particle insertions," *Fluid Phase Equil.*, **83**: 223-231 (1993). DOI: 10.1016/0378-3812(93)87025-V *[10]*
30. E. M. O' Toole and A. Z. Panagiotopoulos, "Effect of sequence and intermolecular interactions on the number and nature of low-energy states for simple model proteins," *J. Chem. Phys.*, **98**: 3185-90 (1993). DOI: 10.1063/1.464091 *[16]*
31. J. R. Recht and A. Z. Panagiotopoulos, "Finite-size effects and approach to criticality in Gibbs ensemble simulations," *Molec. Phys.,* **80**: 843-52 (1993). DOI: 10.1080/00268979300102701 *[62]*
32. J. K. Johnson, A. Z. Panagiotopoulos, and K. E. Gubbins, "Reactive canonical Monte Carlo: A new simulation technique for reacting or associating fluids," *Molec. Phys.,* **81**: 717-733 (1994). DOI: 10.1080/00268979400100481 *[203]*
33. A. Z. Panagiotopoulos, "Molecular simulation of phase equilibria," NATO ASI Series E, **273**, 411-437 (1994). DOI: 10.1007/978-94-015-8295-7_16 *[19]*
34. V. I. Harismiadis, A. Z. Panagiotopoulos, and D. P. Tassios, "Phase equilibria of binary Lennard-Jones mixtures with cubic equations of state," *Fluid Phase Equilibria*, **94:** 1-18 (1994). DOI: 10.1016/0378-3812(94)87049-7 *[23]*
35. Y.-J. Sheng, A. Z. Panagiotopoulos, S. K. Kumar, and I. Szleifer, "Monte Carlo calculation of phase equilibria for a bead-spring polymeric model," *Macromolecules*, **27**: 400-406 (1994). DOI: 10.1021/ma00080a012 *[114]*
36. L. F. Vega, A. Z. Panagiotopoulos, and K. E. Gubbins, "Chemical potentials and adsorption isotherms of polymers confined between parallel plates," *Chem. Eng. Sci.*, **49**, 2921-2929 (1994). DOI: 10.1016/0009-2509(94)E0110-C *[17]*
37. G. Orkoulas and A. Z. Panagiotopoulos, "Free energy and phase equilibria for the restricted primitive model of ionic fluids from Monte Carlo Simulations," *J. Chem. Phys.*, **101**, 1452-59 (1994). DOI: 10.1063/1.467770 *[222]*
38. A. M. Georgoulaki, I. V. Ntouros, D. P. Tassios, and A. Z. Panagiotopoulos, "Phase equilibria of binary Lennard-Jones mixtures: Simulation and van der Waals 1-fluid theory," *Fluid Phase Equil.*, **100**, 153-170 (1994). DOI: 10.1016/0378-3812(94)80007-3 *[59]*
39. A. D. Mackie, A. Z. Panagiotopoulos, D. Frenkel, and S. K. Kumar, "Constant-pressure Monte Carlo simulations for lattice models," *Europhys. Lett.*, **27**, 549-554 (1994). DOI: 10.1209/0295-5075/27/7/010 *[21]*
40. A. Z. Panagiotopoulos, "Monte Carlo simulation of phase coexistence for polymeric and ionic fluids," *Fluid Phase Equil.*, **104**, 185-194 (1995). DOI: 10.1016/0378...02648-K *[7]*
41. E. M. O' Toole, R. Venkataramani, and A. Z. Panagiotopoulos, "A simple lattice model of proteins incorporating directional bonding and a structured solvent," *AIChE J.*, **41**, 954-958 (1995). DOI: 10.1002/aic.690410425 *[5]*
42. A.Z. Panagiotopoulos, "Molecular simulation of phase coexistence: Finite-size effects and determination of critical parameters for two- and three- dimensional Lennard-Jones fluids," *Int. J. Thermophys.*, **15**, 1057-72 (1994). DOI: 10.1007/BF01458815 *[147]*
43. W.T. Gozdz, K.E. Gubbins, and A.Z. Panagiotopoulos, "Liquid-liquid phase transitions in pores," *Molec. Phys.*, **84**, 825-834 (1995). DOI: 10.1080/00268979500100581 *[47]*

44. P. C. Tsang, O. N. White, B. Y. Perigard, L. F. Vega, and A.Z. Panagiotopoulos, "Phase equilibria in ternary Lennard-Jones systems," *Fluid Phase Equil.,* **107**, 31-43 (1995); erratum in **129**, 311 (1997). DOI: 10.1016/0378-3812(94)02628-E *[31]*
45. Y.-J. Sheng, A. Z. Panagiotopoulos, and D.P. Tassios, "Activity coefficients in nearly athermal model polymer/solvent systems," *AIChE J.*, **41**, 2306-13 (1995). DOI: 10.1002/aic.690411014 *[20]*
46. A.D. Mackie, A.Z. Panagiotopoulos, and S.K. Kumar, "Monte Carlo Simulations of Phase Equilibria for a Lattice Homopolymer Model," *J. Chem. Phys.*, **102**, 1014-23 (1995). DOI: 10.1063/1.469450 *[63]*
47. A.Z. Panagiotopoulos, "Gibbs ensemble techniques," NATO ASI Series C, **460**, 463-501 (1995). DOI: 10.1007/978-94-011-0065-6_11 *[66 +10]*
48. Y.-J. Sheng, A.Z. Panagiotopoulos, and S.K. Kumar, "Mixing Properties of Model Polymer/Solvent Systems," *J. Chem. Phys.*, **103**, 10315-24 (1995). DOI: 10.1063/1...9869 *[7]*
49. A.Z. Panagiotopoulos, "Current Advances in Monte Carlo Methods," *Fluid Phase Equil.,* **116**, 257-266 (1996). DOI: 10.1016/0378-3812(95)02894-3 *[35]*
50. Y.-J. Sheng, A.Z. Panagiotopoulos, and S.K. Kumar, "Effect of Chain Stiffness on Polymer Phase Behavior," *Macromolecules,* **29**, 4444-6 (1996). DOI: 10.1021/ma951343y *[37]*
51. A.D. Mackie, K. Onur, and A.Z. Panagiotopoulos, "Phase Equilibria of a lattice model for an oil-water-amphiphile mixture," *J. Chem. Phys.*, **104**, 3718-25 (1996). DOI: 10.1063/1.471026 *[58]*
52. G. Orkoulas and A.Z. Panagiotopoulos, "Phase Diagram of the Two-Dimensional Coulomb Gas: A Thermodynamic Scaling Monte Carlo Study," *J. Chem. Phys.,* **104**, 7205-9 (1996). DOI: 10.1063/1.471406 *[36]*
53. K. Kiyohara, T. Spyrouni, K. E. Gubbins, and A. Z. Panagiotopoulos, "Thermodynamic-Scaling Gibbs Ensemble Monte Carlo: A new method for determination of phase coexistence properties of fluids," *Molec. Phys.,* **89**, 965-74 (1996). DOI: 10.1080/00268979609482517 *[48]*
54. V. I. Harismiadis, J. Vorholz, and A. Z. Panagiotopoulos, "Efficient Pressure Estimation in Molecular Simulations Without Evaluating the Virial," *J. Chem. Phys.,* **105**, 8469-70 (1996). DOI: 10.1063/1.472721 *[84]*
55. C. J. Roberts, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Liquid-liquid Immiscibility in Pure Fluids: Polyamorphism in Simulations of a Network-Forming Pure Fluid," *Phys. Rev. Lett.*, **77**, 4386-9 (1996). DOI: 10.1103/PhysRevLett.77.4386 *[117]*
56. K. Kiyohara, K. E. Gubbins, and A. Z. Panagiotopoulos, "Phase Coexistence Properties of Polarizable Stockmayer Fluids," *J. Chem. Phys.,* **106**, 3338-47 (1997). 10.1063/1.473082 *[50]*
57. A. D. Mackie, A. Z. Panagiotopoulos, and I. Szleifer, "Aggregation Behavior of a Lattice Model for Amphiphiles," *Langmuir*, **13**, 5022-31 (1997). DOI: 10.1021/la961090h *[143]*
58. A.Z. Panagiotopoulos, V. Wong, and M.A. Floriano, "Phase Equilibria of Lattice Polymers from Histogram Reweighting Monte Carlo Simulations," *Macromolecules*, **31**, 912-918 (1998). DOI: 10.1021/ma971108a *[161]*
59. K. Kiyohara, K.E. Gubbins, and A.Z. Panagiotopoulos, "Phase Coexistence Properties of Polarizable Water Models," *Molec. Phys.*, **94**, 803-8 (1998). DOI: 10.1080/0...67638 *[110]*
60. J.R. Errington, K. Kiyohara, K.E. Gubbins and A.Z. Panagiotopoulos, "Monte Carlo simulation of high-pressure phase equilibria in aqueous systems," *Fluid Phase Equil.*, **151**, 33-40 (1998). DOI: 10.1016/S0378-3812(98)00273-8 *[22]*

61. J.R. Errington and A.Z. Panagiotopoulos, "Phase Equilibria of the Modified Buckingham Exponential-6 Potential from Hamiltonian Scaling Grand Canonical Monte Carlo," *J. Chem. Phys.*, **109**, 1093-1100 (1998). DOI: 10.1063/1.476652 *[99]*

62. J.R. Errington, G.C. Boulougouris, I.G. Economou, A.Z. Panagiotopoulos, and D.N. Theodorou, "Molecular Simulation of Phase Equilibria for Water-Methane and Water-Ethane Mixtures," *J. Phys. Chem. B*, **102**, 8865-73 (1998). DOI: 10.1021/jp981627v *[127]*

63. J.R. Errington and A.Z. Panagiotopoulos, "A Fixed Point Charge Model for Water Optimized to the Vapor-Liquid Coexistence Properties," *J. Phys. Chem. B*, **102**, 7470-7475 (1998). DOI: 10.1021/jp982068v *[187]*

64. J.Y. Lee, A.R.C. Baljon, R.F. Loring, and A.Z. Panagiotopoulos, "Simulation of Polymer Melt Intercalation in Layered Nanocomposites," *J. Chem. Phys.*, **109**, 10321-30 (1998). DOI: 10.1063/1.477687 *[65]*

65. G. Orkoulas and A.Z. Panagiotopoulos, "Phase Behavior of the Restricted Primitive Model and Square-Well Fluids from Monte Carlo Simulations in the Grand Canonical Ensemble," *J. Chem. Phys.*, **110**, 1581-90 (1999). DOI: 10.1063/1.477798 *[247]*

66. J.J. Potoff and A.Z. Panagiotopoulos, "Critical point and phase behavior of the pure fluid and a LJ mixture," *J. Chem. Phys.*, **109**, 10914-20 (1998). DOI: 10.1063/ 1.477787 *[367]*

67. M.A. Floriano, E. Caponetti, and A.Z. Panagiotopoulos, "Micellization in Model Surfactant Systems," *Langmuir*, **15**, 3143-3151 (1999). DOI: 10.1021/la9810206 *[205]*

68. J.R. Errington and A.Z. Panagiotopoulos, "A New Intermolecular Potential Model for the n-Alkanes Homologous Series" *J. Phys. Chem. B*, **103**: 6314-22 (1999). DOI: 10.1021/jp990988n *[180]*

69. A.P. Chatterjee and A.Z. Panagiotopoulos, "Monte Carlo Simulations of Model Nonionic Surfactants," Springer Proceeding in Physics **85**: 211-222 (1999). DOI: 10.1007/...9-6_21

70. S. K. Kumar and A. Z. Panagiotopoulos, "Thermodynamics of Reversibly Associating Polymer Solutions," *Phys. Rev. Lett.* **82**: 5060-3 (1999). 10.1103/PhysRevLett.82.5060 *[62]*

71. J. J. Potoff, J. R. Errington, and A. Z. Panagiotopoulos, "Molecular Simulation of Phase Equilibria for Mixtures of Polar and Non-Polar Components," *Molec. Phys.*, **97**, 1073-85 (1999). DOI: 10.1080/00268979909482908 *[155]*

72. A. Z. Panagiotopoulos, "Monte Carlo Methods for Phase Equilibria," *J. Phys. Condensed Matter*, **12**, R25-R52 (2000). DOI: 10.1088/0953-8984/12/3/201 *[301+29]*

73. A.Z. Panagiotopoulos and S. K. Kumar, "Large Lattice Discretization Effects on the Phase Coexistence of Ionic Fluids," *Phys. Rev. Lett.*, **83**, 2981-4 (1999). DOI: 10.1103/PhysRevLett.83.2981 *[107]*

74. J. R. Errington and A. Z. Panagiotopoulos, "New Intermolecular Potential Models for Benzene and Cyclohexane," *J. Chem. Phys.*, **111**, 9731-8 (1999). DOI: 10.1063/1.480308 *[115]*

75. N. Gilra, C. Cohen, and A. Z. Panagiotopoulos, "A Monte Carlo study of the structural properties of end-linked polymer networks," *J. Chem. Phys.*, **112**, 6910-6 (2000). DOI: 10.1063/1.481264 *[61]*

76. G. Orkoulas, A. Z. Panagiotopoulos, and M. E. Fisher, "Criticality and crossover in accessible regimes," *Phys. Rev. E*, **61**, 5930-9 (2000).). DOI: 10.1103/PhysRevE.61.5930 *[48]*

77. A. Z. Panagiotopoulos, "On the equivalence of continuum and lattice models for fluids," *J. Chem. Phys.*, **112**, 7132-7 (2000). DOI: 10.1063/1.481307 *[85]*

78. G. C. Boulougouris, J. R. Errington, I. G. Economou, A. Z. Panagiotopoulos, and D. N. Theodorou, "Molecular simulation of phase equilibria for water–n-butane and water–n-hexane mixtures," *J. Phys. Chem. B*, **104**, 4958-63 (2000). DOI: 10.1021/jp994063j *[49]*

79. J. Vorholz, V. I. Harismiadis, B. Rumpf, A. Z. Panagiotopoulos, and G. Maurer, "Vapor-Liquid Equilibrium of Water, Carbon Dioxide and the Binary System Water + Carbon Dioxide from Molecular Simulation," *Fluid Phase Equil.*, **170**, 203-34 (2000). DOI: 10.1016/S0378-3812(00)00315-0 *[159]*

80. J. Potoff and A. Z. Panagiotopoulos, "Surface tension of the 3-dimensional Lennard-Jones fluid from histogram-reweighting Monte Carlo simulations," J. Chem. Phys., **112**, 6411-5 (2000). DOI: 10.1063/1.481204 *[159]*

81. A. Z. Panagiotopoulos, "Force Field Development for Simulations of Condensed Phases," *AIChE Symp. Ser. No. 325,* **97**, 61-70 (2001). *[3]*

82. S. K. Kumar, M. A. Floriano, and A. Z. Panagiotopoulos, "Nanostructure Formation and Phase Separation in Surfactant Solutions," *Adv. Chem. Eng.*, **28**, 297-311 (2001).

83. J. M. Romero-Enrique, G. Orkoulas, A. Z. Panagiotopoulos, and M. E. Fisher, "Coexistence and Criticality in Size-Asymmetric Hard-Core Electrolytes," *Phys. Rev. Lett.* **85**, 4558-61 (2000). DOI: 10.1103/PhysRevLett.85.4558 *[115]*

84. E. Luijten, M. E. Fisher, and A. Z. Panagiotopoulos, "The heat capacity of the restricted primitive model electrolyte," *J. Chem. Phys.*, **114**, 5468-71 (2001). *[30 +3]*

85. G. Orkoulas, M. E. Fisher & A. Z. Panagiotopoulos, "Precise simulation of criticality in asymmetric fluids," *Phys. Rev. E,* **63**, 051507 (2001). DOI: 10.1103/PhysRevE.63.051507 *[115]*

86. N. Gilra, A. Z. Panagiotopoulos, and C. Cohen, "Monte Carlo simulations of free chains in end-linked polymer networks," *J. Chem. Phys.,* **115**, 1100-1104 (2001). DOI: 10.1063/1.1379573 *[15]*

87. N. Gilra, A. Z. Panagiotopoulos, and C. Cohen, "Monte Carlo Simulations of Polymer Network Deformation," *Macromolecules,* **34**, 6090-6 (2001). DOI: 10.1021/ma0021895 *[17]*

88. N. Gilra, C. Cohen, R. M. Briber, B. J. Bauer, and A. Z. Panagiotopoulos, "A SANS study of the conformational behavior of linear chains in strained and unstrained end-linked elastomers," *Macromolecules,* **34**, 7773-82 (2001). DOI: 10.1021/ma010018+ *[24]*

89. M. Lísal, C. K. Hall, K. E. Gubbins, and A. Z. Panagiotopoulos, "Self-Assembly of surfactants in a supercritical solvent from lattice Monte Carlo simulations," *J. Chem. Phys*, **116**, 1171-84 (2002). DOI: 10.1063/1.1428347 *[57]*

90. A. Z. Panagiotopoulos and M. E. Fisher, "Phase Transitions in 2:1 and 3:1 Hard-Core Model Electrolytes," *Phys. Rev. Lett.*, **88**, 045701 (2002). DOI: 10.1103/...88.045701 *[62]*

91. S.-Y. Kim, A. Z. Panagiotopoulos, and M. A. Floriano, "Ternary Oil-Water-Amphiphile Systems: Self-Assembly and Phase Equilibria," *Molec. Phys.*, **100**, 2213-2220 (2002). DOI: 10.1080/00268970210125331 *[34]*

92. A. Z. Panagiotopoulos, "Gibbs-Ensemble and Histogram-Reweighting Grand Canonical Monte Carlo Methods," chapter 9 in *Simulation Methods for Polymers*, D. N. Theodorou and A. Kotalyanskii (eds.), Marcel Dekker, 2004 (pp. 313-344).

93. A. Indrakanti, J. K. Maranas, A. Z. Panagiotopoulos, and S. K. Kumar, "Quantitative Lattice Simulations of the Structure and Thermodynamics of Macromolecules," *Macromolecules,* **34**, 8596-99 (2001). DOI: 10.1021/ma011379s *[11]*

94. A. Z. Panagiotopoulos, "Critical Parameters of the Restricted Primitive Model," *J. Chem. Phys.*, **116**, 3007-11 (2002). DOI: 10.1063/1.1435571 *[88]*

95. M. Lísal, C. K. Hall, K. E. Gubbins, and A. Z. Panagiotopoulos, "Micellar Behavior in Supercritical Solvent-Surfactant Systems from Lattice Monte Carlo Simulations," *Fluid Fluid Phase Equilibria*, **194**, 233-47 (2002). DOI: 10.1016/S0378-3812(01)00721-X *[21]*

96. E. Luijten, M. E. Fisher, and A. Z. Panagiotopoulos, "Universality Class of Criticality in the Restricted Primitive Model Electrolyte," *Phys. Rev. Lett.*, **88**, 185701 (2002). DOI: 10.1103/PhysRevLett.88.185701 *[176]*

97. A. Z. Panagiotopoulos, M. A. Floriano, and S. K. Kumar, "Micellization and Phase Separation of Diblock and Triblock Model Surfactants," *Langmuir*, **18**(7), 2940-48 (2002). DOI: 10.1021/la0156513 *[126]*

98. L. X. Dang, T.-M. Chang, and A. Z. Panagiotopoulos, "Gibbs ensemble Monte Carlo simulations of coexistence properties of a polarizable potential model of water," *J. Chem. Phys.* **117**, 3522-3, (2002). DOI: 10.1063/1.1493190 *[23]*

99. A. G. Makeev, D. Maroudas, A. Z. Panagiotopoulos, and I. G. Kevrekidis, "Coarse Bifurcation Analysis of Kinetic Monte Carlo Simulations," *J. Chem. Phys.* **117**, 8229-40 (2002). DOI: 10.1063/1.1512274 *[85]*

100. M. S. Shell, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Molecular structural order and anomalies in liquid silica," *Phys. Rev. E* **66**, 011202 (2002). DOI: 10.1103/ PhysRevE.66.011202 *[236]*

101. M. S. Shell, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Generalization of the Wang-Landau method for off-lattice simulations," *Phys. Rev. E,* **66**, 056703 (2002). DOI: 10.1103/PhysRevE.66.056703 *[204]*

102. S. Salaniwal, S. K. Kumar, and A. Z. Panagiotopoulos, "Competing Ranges of Attractive and Repulsive Interactions in the Micellization of Model Surfactants," *Langmuir,* **19**(12) 5164-5168 (2003). DOI: 10.1021/la026076l *[27]*

103. J. M. Romero-Enrique, L. F. Rull, and A. Z. Panagiotopoulos, "Dipolar origin of the gas-liquid coexistence of the hard-core 1:1 electrolyte model," *Phys. Rev. E,* **66**, 041204 (2002). DOI: 10.1103/PhysRevE.66.041204 *[37]*

104. G. Orkoulas, S. K. Kumar, and A. Z. Panagiotopoulos, "Monte Carlo Study of Coulombic Criticality in Polyelectrolytes," *Phys. Rev. Lett.,* **90**, 048303 (2003). DOI: 10.1103/PhysRev Lett.90.048303 *[54]*

105. M. Lísal, C. K. Hall, K. E. Gubbins, and A. Z. Panagiotopoulos, "Formation of spherical micelles in a supercritical solvent: Lattice Monte Carlo simulation and multicomponent solution model," *Molec. Simulation*, **29**, 139-157 (2003). DOI: 10.1080/...0065809 *[7]*

106. A. Diehl and A. Z. Panagiotopoulos, "Phase transitions and tricriticality in the lattice restricted primitive model supplemented by short-range interactions," *J. Chem. Phys.* **118**, 4993-8 (2003). DOI: 10.1063/1.1545095 *[20]*

107. S. Moghaddam and A. Z. Panagiotopoulos, "Lattice discretization effects on the critical parameters of model nonpolar and polar fluids," *J. Chem. Phys.*, **118**, 7556-61 (2003). DOI: 10.1063/1.1562613 *[9]*

108. M. S. Shell, P. G. Debenedetti, and A. Z. Panagiotopoulos, "An improved Monte Carlo method for direct calculation of the density of states," *J. Chem. Phys.*, **119**, 9406-11 (2003). DOI: 10.1063/1.1615966 *[136]*

109. O. M. Suleimenov, A. Z. Panagiotopoulos, and T. M. Seward, "Grand canonical Monte Carlo simulations of phase equilibria of pure silicon tetrachloride and its binary mixture with carbon dioxide," *Molec. Phys.*, **101**, 3213-3223 (2003). DOI: 10.1080/...624524 *[8]*

110. D. W. Cheong and A. Z. Panagiotopoulos, "Critical parameters of unrestricted primitive model electrolytes with charge asymmetries up to 10:1," *J. Chem. Phys.,* **119**, 8526-8536 (2003). DOI: 10.1063/1.1612473 *[37]*

111. V. Kobelev, A. B. Kolomeisky, and A. Z. Panagiotopoulos, "Thermodynamics of electrolytes on anisotropic lattices," *Phys. Rev. E,* **68**, 066110 (2003). DOI: 10.1103/PhysRevE.68.066110 *[6]*
112. M. S. Shell, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Saddles in the Energy Landscape: Extensivity and Thermodynamic Formalism," *Phys. Rev. Lett.*, **92,** 035506 (2004); Erratum in *Phys. Rev. Lett.*, **92,** 169902. DOI: 10.1103/PhysRevLett.92.035506 *[26]*
113. J. Vorholz, V. I. Harismiadis, A. Z. Panagiotopoulos, B. Rumpf, and G. Maurer, "Molecular simulation of the solubility of carbon dioxide in aqueous solutions of sodium chloride," *Fluid Phase Equil,* **226**, 237-250 (2004). DOI: 10.1016/j.fluid.2004.09.009 *[37]*
114. O. J. Hehmeyer, G. Arya, A. Z. Panagiotopoulos, "Phase Transitions of Confined Lattice Homopolymers," *J. Phys. Chem. B*, **108**, 6809-6815 (2004). DOI: 10.1021/jp037599k *[16]*
115. G. Arya and A. Z. Panagiotopoulos, "Monte Carlo study of shear-induced alignment of cylindrical micelles in thin films," *Phys. Rev. E*, **70**, 031501 (2004). DOI: 10.1103/PhysRevE.70.031501 *[23]*
116. S. Moghaddam and A. Z. Panagiotopoulos, "Determination of second virial coefficients by grand canonical Monte Carlo simulations," *Fluid Phase Equil.*, **222-3**, 221-4 (2004). *[7]*
117. C. S. Lock, S. Moghaddam, and A. Z. Panagiotopoulos, "Finely discretized lattice simulations of SPC/E water," *Fluid Phase Equil.*, **222-3**, 225-30 (2004). *[1]*
118. D. I. Kopelevich, A. Z. Panagiotopoulos, and I. G. Kevrekidis, "Coarse-grained computations for a micellar system," *J. Chem. Phys.*, **122**, 044907, 14pp (2005). DOI: 10.1063/1.1839173 *[24]*
119. D. I. Kopelevich, A. Z. Panagiotopoulos, and I. G. Kevrekidis, "Coarse-grained kinetic computations for rare events: application to micelle formation," *J. Chem. Phys.*, **122**, 044908, 13pp (2005). DOI: 10.1063/1.1839174 *[75]*
120. M. S. Shell, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Flat-histogram dynamics and optimization in density of states simulations of fluids," *J. Phys. Chem. B*, **108**, 19748-55 (2004). DOI: 10.1021/jp047677j *[32]*
121. M. A. Floriano, V. Firetto, and A. Z. Panagiotopoulos, "Effect of stiffness on the phase behavior of cubic lattice chains," *Macromolecules*, **38**, 2475-81 (2005). DOI: 10.1021/ma047671s *[10]*
122. A. Diehl and A. Z. Panagiotopoulos, "Phase diagrams in the lattice restricted primitive model: From order-disorder to gas-liquid phase transition," *Phys. Rev. E.,* **71**, 046118, 7 pp (2005). DOI: 10.1103/PhysRevE.71.046118 *[11]*
123. G. Arya and A. Z. Panagiotopoulos, "Molecular modeling of shear-induced alignment of cylindrical micelles," *Comp. Phys. Comm.*, **169**, 262-266 (2005). *[10]*
124. D. W. Cheong and A. Z. Panagiotopoulos, "Phase Behavior of Polyampholyte Chains from Grand Canonical Monte Carlo Simulations," *Molec. Phys.*, **103**, 3031-44 (2005). DOI: 10.1080/00268970500186045 *[23]*
125. A.-P. Hynninen, M. Dijkstra, and A. Z. Panagiotopoulos, "Critical Point of Electrolyte Mixtures," *J. Chem. Phys.*, **123**, 084903, 9 pp (2005). DOI: 10.1063/1.1979490 *[26]*
126. A. Z. Panagiotopoulos, "Thermodynamic properties of lattice hard sphere models," *J. Chem. Phys.*, **123**, 104504, 5 pp (2005). DOI: 10.1063/1.2008253 *[36]*
127. A. Z. Panagiotopoulos, "Simulations of phase transitions in ionic systems," *J. Phys.: Condens. Matter*, **17**, S3205-13 (2005). DOI: 10.1088/0953-8984/17/45/003 *[18]*
128. G. Arya and A. Z. Panagiotopoulos, "Log-rolling micelles in sheared block copolymer thin films," *Phys. Rev. Lett.*, **95**, 188301, 4 pp (2005). DOI: 10.1103/PhysRevLett.95.188301 *[21]*

129. G. Arya and A. Z. Panagiotopoulos, "Impact of branching on the phase behavior of polymers," *Macromolecules*, **38**, 10596-604 (2005). DOI: 10.1021/ma0515376 *[27]*

130. G. Arya, J. Rottler, A. Z. Panagiotopoulos, D. J. Srolovitz, and P. M. Chaikin, "Shear Ordering in Thin Films of Spherical Block Copolymer Micelles," *Langmuir*, **21**, 11518-27 (2005). DOI: 10.1021/la0516476 *[32]*

131. Y. C. Kim, M. E. Fisher, and A. Z. Panagiotopoulos, "Universality of ionic criticality: Size- and charge-asymmetric electrolytes," *Phys. Rev. Lett.*, **95**, 195703, 4 pp, (2005). DOI: 10.1103/PhysRevLett.95.195703 *[32]*

132. M. S. Shell, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Computational characterization of the sequence landscape in simple protein alphabets," *Proteins*, **62**: 232-243 (2006). DOI: 10.1002/prot.20714 *[10]*

133. M. S. Shell, P. G. Debenedetti, and A. Z. Panagiotopoulos, "A conformal solution theory for the energy landscape and glass transition of mixtures," *Fluid Phase Equil.,* **241**: 147-154 (2006). DOI: 10.1016/j.fluid.2005.11.002 *[15]*

134. C.-Y. Chou, T. T. M. Vo, A. Z. Panagiotopoulos, and M. Robert, "Computer simulations of phase transitions of bulk and confined colloid-polymer systems," *Physica A*, **369**: 275-290 (2006). DOI: 10.1016/j.physa.2006.01.079 *[21]*

135. D. W. Cheong and A. Z. Panagiotopoulos, "Monte Carlo Simulations of Micellization in Model Ionic Surfactants: Application to Sodium Dodecyl Sulfate," *Langmuir*, **22**: 4076-83 **(**2006). DOI: 10.1021/la053511d *[50]*

136. A. Diehl and A. Z. Panagiotopoulos, "Phase behavior of the Lattice Restricted Primitive Model with nearest-neighbor exclusion," *J. Chem. Phys.*, **124**: 194509, 6 pp (2006). *[5]*

137. P. J. Lenart and A. Z. Panagiotopoulos, "Phase Behavior of Binary Stockmayer and Polarizable Lennard-Jones Fluid Mixtures Using Adiabatic Nuclear and Electronic Sampling," *Ind. Eng. Chem. Research*, **45**: 6929-6938 (2006). DOI: 10.1021/ie051302i *[7]*

138. V. Firetto, M. A. Floriano, and A. Z. Panagiotopoulos, "Effect of stiffness on the micellization behavior of model H_4T_4 surfactant chains," *Langmuir*, **22**: 6514-22 (2006). DOI: 10.1021/la060386c *[25]*

139. A.-P. Hynninen, A. Z. Panagiotopoulos, M. C. Rechtsman, F. H. Stillinger, and S. Torquato, "Global phase diagram for the honeycomb potential", *J. Chem. Phys.*, **125**: 024505, 5 pp (2006). DOI: 10.1063/1.2213611 *[9]*

140. P. J. Lenart and A. Z. Panagiotopoulos, "Tracing the Critical Loci of Binary Fluid Mixtures," *J. Phys. Chem. B*, **110**: 17200-6 (2006). DOI: 10.1021/jp0630931 *[7]*

141. J. R. Davis, M. V. Piccarreta, R. B. Rauch, T. K. Vanderlick, and A. Z. Panagiotopoulos, "Phase Behavior of Rigid Objects on a Cubic Lattice," *Ind. Eng. Chem. Res.*, **45**: 5421-5425 (2006). DOI: 10.1021/ie051041c *[3]*

142. A. N. Rissanou, I. G. Economou, and A. Z. Panagiotopoulos, "Monte Carlo simulation of the phase behavior of model dendrimers," *Macromolecules*, **39**: 6298-6305 (2006). DOI: 10.1021/ma061339u *[17]*

143. P. J. Lenart, A. Jusufi, and A. Z. Panagiotopoulos, "Effective potentials for 1:1 electrolyte solutions incorporating dielectric saturation and repulsive hydration," *J. Chem. Phys.*, **126**: 044509, 7 pp (2007). DOI: 10.1063/1.2431169 *[74]*

144. A.-P. Hynninen and A. Z. Panagiotopoulos, "Disappearance of the gas-liquid phase transition for highly charged colloids," *Phys. Rev. Lett.*, **98**: 198301 (2007). DOI: 10.1103/PhysRevLett.98.198301 *[25]*

145. O. J. Hehmeyer, G. Arya, A. Z. Panagiotopoulos, and I. Szleifer, "Monte Carlo simulation and molecular theory of tethered polyelectrolytes," *J. Chem. Phys.*, **126**: 244902 (2007). DOI: 10.1063/1.2747600 *[47]*

146. M. E. Gindy, A. Z. Panagiotopoulos, and R. K. Prud'homme, "Composite block copolymer stabilized nanoparticles: Simultaneous encapsulation of organic actives and inorganic nanostructures," *Langmuir*, **24**: 83-90 (2008). DOI: 10.1021/la702902b *[201]*

147. M. Sammalkorpi, A. Z. Panagiotopoulos, and M. Haataja, "Structure and dynamics of surfactant and hydrocarbon aggregates on graphite: a molecular dynamics simulation study," *J. Phys. Chem. B*, **112**: 2915-21 (2008). DOI: 10.1021/jp077636y *[50]*

148. M. E. Gindy, R. K. Prud'homme, and A. Z. Panagiotopoulos, "Phase behavior and structure formation in linear multiblock copolymer solutions by Monte Carlo simulation," *J. Chem. Phys.,* **128**: 164906 (2008). DOI: 10.1063/1.2905231 *[37]*

149. M. E. Gindy, S. Ji, T. R. Hoye, A. Z. Panagiotopoulos, and R. K.Prud'homme, "Preparation of polyethylene glycol protected nanoparticles with variable bioconjugate ligand density," *Biomacromolecules,* **9**: 2705-2711 (2008). DOI: 10.1021/bm8002013 *[137]*

150. M. Sammalkorpi, A. Z. Panagiotopoulos, and M. Haataja, "Surfactant and hydrocarbon aggregates on defective graphite surface: structure and dynamics," *J. Phys. Chem. B,* **112**: 12954-61 (2008). DOI: 10.1021/jp8043835 *[30]*

151. A. Jusufi, A.-P. Hynninen, and A. Z. Panagiotopoulos, "Implicit-solvent Models for Micellization of Ionic Surfactants," *J. Phys. Chem. B,* **112**: 13783-92 (2008). DOI: 10.1021/jp8043225 *[65]*

152. A.-P. Hynninen and A. Z. Panagiotopoulos, "Invited topical review: Simulations of phase transitions and free energies for ionic systems," *Molec. Phys.* **106**: 2039-2051 (2008). DOI: 10.1080/00268970802112160 *[38]*

153. J. R. Davis, A. Z. Panagiotopoulos, "Monte Carlo simulations of amphiphilic nanoparticle self-assembly," *J. Chem. Phys.* **129**: 194706, 7 pp (2008). DOI: 10.1063/ 1.3009183 *[18]*

154. T. Chen, A.-P. Hynninen, R. K. Prud'homme, I. G. Kevrekidis, and A. Z. Panagiotopoulos, "Coarse-grained simulations of rapid assembly kinetics for polystyrene-b-poly(ethylene oxide) copolymers in aqueous solutions," *J. Phys. Chem. B,* **112**: 16357-16366 (2008). DOI: 10.1021/jp805826a *[52]*

155. T. Chen, S. M. D'Addio, M. T. Kennedy, A. Swietlow, I. G. Kevrekidis, A. Z. Panagiotopoulos, and R. K. Prud'homme, "Protected peptide nanoparticles: Experiments and Brownian dynamics simulations of the energetics of assembly," *Nano Lett.,* **9**: 2218-2222 (2009). DOI: 10.1021/nl803205c *[52]*

156. F. Lo Verso, A. Z. Panagiotopoulos, and C. N. Likos, "Aggregation phenomena in telechelic star polymer solutions," *Phys. Rev. E*, **79**: 010401, (2009). DOI: 10.1103/PhysRevE.79.010401 *[29]*

157. P. Akcora, H. Liu, S. K. Kumar, J. Moll, Y. Li, B. C. Benicewicz, L. S. Schadler, D. Acehan, A. Z. Panagiotopoulos, V. Pryamitsyn, V. Ganesan, J. Ilavsky, P. Thiyagarajan, R. H. Colby, and J. F. Douglas, "Anisotropic self-assembly of spherical polymer-grafted nanoparticles," *Nature Mater.*, **8**: 354-359 (2009). DOI: 10.1038/nmat2404 *[1,035]*

158. A. Jusufi, A.-P. Hynninen, M. Haataja, and A. Z. Panagiotopoulos, "Electrostatic screening and charge correlation effects in micellization of ionic surfactants," *J. Phys. Chem. B.*, **113**: 6314-6320 (2009). DOI: 10.1021/jp901032g *[54]*

159. A. L. Ferguson, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Solubility and molecular conformations of n-alkane chains in water," *J. Phys. Chem. B.*, **113**: 6405-6414 (2009). DOI: 10.1021/jp811229q *[155]*

160. F. Lo Verso, A. Z. Panagiotopoulos, and C. N. Likos, "Phase behavior of low-functionality, telechelic star block copolymers," *J. Chem. Soc. Faraday Disc.,* **144**: 143-157 (2010). DOI: 10.1039/b905073f *[14]*

161. Y. Liu, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Low Temperature Fluid-Phase Behavior of ST2 Water," J. *Chem. Phys.*, **131**: 104508, 7 pp (2009). 10.1063/1.3229892 *[157]*

162. J. R. Davis and A. Z. Panagiotopoulos, "Micellization and phase separation in binary amphiphile mixtures," *Molec. Phys.*, **107**: 2359-66 (2009). DOI: 10.1080/...79017 *[16]*

163. A. Z. Panagiotopoulos, "Charge correlation effects on ionization of weak polyelectrolytes," *J. Phys. Condens. Matter*, **21**: 424113, 7 pp (2009). DOI: 10.1088/.../42/424113 *[40]*

164. J. R. Davis and A. Z. Panagiotopoulos, "Orientational bonding model for temperature dependent micellization and solubility of diblock surfactants," *J. Chem. Phys.*, **131**: 114901, 5 pp (2009). DOI: 10.1063/1.3227905 *[4]*

165. A.-P. Hynninen and A. Z. Panagiotopoulos, "Phase diagrams of charged colloids from thermodynamic integration," *J. Phys. Condens. Matter*, **21**: 465104, 7 pp (2009). DOI: 10.1088/0953-8984/21/46/465104 *[6]*

166. V. Pryamtisyn, V. Ganesan, A. Z. Panagiotopoulos, H. Liu, and S. K. Kumar, "Modeling the anisotropic self-assembly of spherical polymer-grafted nanoparticles," *J. Chem. Phys.* **131**: 221102, 4 pp (2009). DOI: 10.1063/1.3267729 *[133]*

167. S. Sanders and A. Z. Panagiotopoulos, "Micellization behavior of coarse-grained surfactant models," *J. Chem. Phys.,* **132**: 114902, 9 pp (2010). DOI: 10.1063/1.3358354 *[81]*

168. Y. Liu, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Finite-size scaling study of the vapor-liquid critical properties of confined fluids: Crossover from three dimensions to two dimensions," *J. Chem. Phys.,* **132**: 144107, 10 pp (2010). DOI: 10.1063/1.3377089 *[29]*

169. A. Chremos, K. Margaritis, and A. Z. Panagiotopoulos, "Ultra thin films of diblock copolymers under shear," *Soft Matter,* **6**: 3588-3595 (2010). DOI: 10.1039/c003198d *[25]*

170. A. L. Ferguson, A. Z. Panagiotopoulos, P. G. Debenedetti, and I. G. Kevrekidis, "Systematic determination of order parameters for chain dynamics using diffusion maps," *Proc. Natl. Acad. Sci. USA*, **107**: 13597-602 (2010). DOI: 10.1073/pnas.1003293107 *[167]*

171. B. Hong, F. Escobedo, and A. Z. Panagiotopoulos, "Diffusivities and Viscosities of Poly(ethylene oxide) Oligomers," *J. Chem. Eng. Data,* **55**: 4273-4280 (2010). DOI: 10.1021/je100430q *[14]*

172. A. L. Ferguson, S. Zhang, I. Dikiy, A. Z. Panagiotopoulos, P. G. Debenedetti, and A. J. Link, "An Experimental and Computational Investigation of Spontaneous Lasso Formation in Microcin J25," *Biophys. J.*, **99**: 3056-3065 (2010). DOI: 10.1016/ j.bpj.2010.08.073 *[64]*

173. J. R. Spaeth, T. Dale, I. G. Kevrekidis, and A. Z. Panagiotopoulos, "Coarse-Graining of Chain Models in Dissipative Particle Dynamics Simulations," *Ind. Eng. Chem. Res.*, **50**: 69-77 (2011). DOI: 10.1021/ie100337r *[30]*

174. A. Jusufi, S. Sanders, M. L. Klein, and A. Z. Panagiotopoulos, "Implicit-Solvent Models for Micellization: Nonionic Surfactants and Temperature-Dependent Properties," *J. Phys. Chem. B*, **115**: 990-1001 (2011). DOI: 10.1021/jp108107f *[28]*

175. M. Sammalkorpi, S. Sanders, A. Z. Panagiotopoulos, M. Karttunen, and M. Haataja, "Simulations of micellization of sodium hexyl sulfate", *J. Phys. Chem. B* **115**: 1403-1410 (2011). DOI: 10.1021/jp109882r *[39]*

176. A. L. Ferguson, A. Z. Panagiotopoulos, P. G. Debenedetti, and I. G. Kevrekidis, "Integrating diffusion maps with umbrella sampling: Application to alanine dipeptide," *J. Chem. Phys*., **134**: 135103, 15 pp (2011). DOI: 10.1063/1.3574394 *[80]*

177. J. R. Spaeth, I. G. Kevrekidis, and A. Z. Panagiotopoulos, "A Comparison of Implicit- and Explicit-Solvent Simulations of Self-Assembly in Block Copolymer and Solute Systems," *J. Chem. Phys.*, **134**: 164902, 13 pp (2011). DOI: 10.1063/1.3580293 *[76]*

178. J. C. Araque, A. Z. Panagiotopoulos, and M. A. Robert, "Lattice Model of Oligonucleotide Hybridization in Solution: I. Model and Thermodynamics," *J. Chem. Phys.*, **134**: 165103, 14 pp (2011). DOI: 10.1063/1.3568145 *[17]*

179. Y. Liu, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Monte Carlo Simulations of High-Pressure Phase Equilibria of CO2–H2O Mixtures," *J. Phys. Chem. B*, **115**: 6629-35 (2011). DOI: 10.1021/jp201520u *[50]*

180. A. L. Ferguson, A. Z. Panagiotopoulos, I. G. Kevrekidis, and P. G. Debenedetti, "Nonlinear dimensionality reduction in molecular simulation: The diffusion map approach," *Chem. Phys. Lett.*, **509**: 1-11 (2011). DOI: 10.1016/j.cplett.2011.04.066 *[156]*

181. S. A. Barr and A. Z. Panagiotopoulos, "Interactions Between Charged Surfaces with Ionizable Sites," *Langmuir*, **27**: 8761-66 (2011). DOI: 10.1021/la201353u *[21]*

182. A. Chremos and A. Z. Panagiotopoulos, "Structural transitions of solvent-free oligomer-grafted nanoparticles," *Phys. Rev. Lett.*, **107**: 105503, 5 pp (2011). DOI: 10.1103/PhysRevLett.107.105503 *[59]*

183. B. Hong, A. Chremos, and A. Z. Panagiotopoulos, "Simulations of the structure and dynamics of nanoparticle-based ionic liquids," *Faraday Disc.*, **154**: 29-40 (2012). DOI: 10.1039/c1fd00076d *[24]*

184. A. Chremos, A. Z. Panagiotopoulos, H.-Y. Yu, and D. L. Koch, "Structure of solvent-free grafted nanoparticles: Molecular dynamics and density-functional theory," *J. Chem. Phys.*, **135**: 114901, 12 pp (2011). DOI: 10.1063/1.3638179 *[46]*

185. C. Koch, C. N. Likos, A. Z. Panagiotopoulos, and F. LoVerso, "Self-assembly scenarios of block copolymer stars," *Molec. Phys.* **109**: 3049-60 (2011). DOI: 10.1080/00268...27385 *[13]*

186. J. R. Spaeth, I. G. Kevrekidis, and A. Z. Panagiotopoulos, "Dissipative Particle Dynamics Simulations of Polymer-protected Nanoparticle Self-Assembly," *J. Chem. Phys.*, **135**: 184903, 10 pp (2011). DOI: 10.1063/1.3653379 *[42]*

187. D. N. LeBard, B. G. Levine, P. Mertmann, S. A. Barr, A. Jusufi, S. Sanders, M. L. Klein, and A. Z. Panagiotopoulos, "Self-assembly of coarse-grained ionic surfactants accelerated by graphics processing units," *Soft Matter*, **8**: 2385-97 (2012). DOI: 10.1039/c1sm06787g *[136]*

188. A. Chremos, A. Z. Panagiotopoulos, and D. L. Koch, "Dynamics of solvent-free grafted nanoparticles," *J. Chem. Phys.*, **136**: 044902, 9 pp (2012). DOI: 10.1063/1.3679442 *[49]*

189. S. Sanders, M. Sammalkorpi, and A. Z. Panagiotopoulos, "Atomistic Simulations of Micellization of Sodium Hexyl, Heptyl, Octyl and Nonyl Sulfates," *J. Phys. Chem. B*, **116**: 2430-37 (2012). DOI: 10.1021/jp209207p *[89]*

190. B. Hong and A. Z. Panagiotopoulos, "Molecular Dynamics Simulations of Silica Nanoparticles grafted with Poly(Ethylene Oxide) Oligomer Chains," *J. Phys. Chem. B*, **116**: 2385-95 (2012). DOI: 10.1021/jp2112582 *[62]*

191. A. Chremos, P. M. Chaikin, R. A. Register, and A. Z. Panagiotopoulos, "Sphere-to-cylinder transitions in thin films of diblock copolymers under shear," *Macromolecules*, **45**: 4406-15 (2012). DOI: 10.1021/ma300382v *[26]*

192. N. A. Mahynski, T. Lafitte, and A. Z. Panagiotopoulos, "Pressure and density scaling for colloid-polymer systems in the protein limit," *Phys. Rev. E*, **85**: 051402, 9 pp (2012). DOI: 10.1103/PhysRevE.85.051402 *[15]*
193. B. Hong, A. Chremos, and A. Z. Panagiotopoulos, "Dynamics in coarse-grained models for oligomer-grafted silica nanoparticles," *J. Chem. Phys.* **136**: 204904, 9 pp (2012). DOI: 10.1063/1.4719957 *[25]*
194. K. B. Daly, J. B. Benziger, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Massively parallel chemical potential calculation on graphics processing units," *Comp. Phys. Comm.*, **183**: 2054-62 (2012). DOI: 10.1016/j.cpc.2012.05.006 *[23]*
195. S. A Barr and A. Z. Panagiotopoulos, "Grand Canonical Monte Carlo Method for Donnan Equilibria," *Phys. Rev. E*, **86**: 016703, 5 pp (2012). DOI: 10.1103/PhysRevE.86.016703 *[12]*
196. A. Chremos, P. M. Chaikin, R. A. Register, and A. Z. Panagiotopoulos, "Shear-induced Alignment of Lamellae in Thin Films of Diblock Copolymers," *Soft Matter* **8**: 7803-7811 (2012). DOI: 10.1039/c2sm25592h *[21]*
197. A. L. Ferguson, N. Giovambattista, P. J. Rossky, A. Z. Panagiotopoulos, and P. G. Debenedetti, "A Computational Investigation of the Phase Behavior and Capillary Sublimation of Water Confined Between Nanoscale Hydrophobic Plates," *J. Chem. Phys.* **137**: 144501, 21 pp (2012) [Cover article]. DOI: 10.1063/1.4755750 *[46]*
198. S. A. Barr, A. Z. Panagiotopoulos, "Conformational transitions of weak polyacids grafted to nanoparticles," *J. Chem. Phys.,* **137**: 144704, 6 pp. (2012). DOI: 10.1063/1.4757284 *[20]*
199. Y. Liu, J. C. Palmer, A. Z. Panagiotopoulos, P. G. Debenedetti, "Liquid-liquid transition in ST2 water," *J. Chem. Phys.,* **137**: 214505, 10 pp. (2012). DOI: 10.1063/ 1.4769126 *[157]*
200. Y. Liu, T. Lafitte, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Simulations of Vapor–Liquid Phase Equilibrium and Interfacial Tension in the CO_2–H_2O–NaCl System," *AIChE J.*, **59**: 3514-22 (2013). DOI: 10.1002/aic.14042 *[45]*
201. N. A. Mahynski, B. Irick, and A. Z. Panagiotopoulos, "Structure of Phase-Separated Athermal Colloid-Polymer Systems in the Protein Limit," *Phys. Rev. E*, **87**: 022309, 9 pp (2013). DOI: 10.1103/PhysRevE.87.022309 *[15]*
202. B. Hong and A. Z. Panagiotopoulos, "Diffusivities, viscosities, and conductivities of solvent-free ionically grafted nanoparticles," *Soft Matter*, **9**: 6091-6102 (2013). DOI: 10.1039/C3SM50832C *[10]*
203. C. Koch, A. Z. Panagiotopoulos, F. Lo Verso, and C. N. Likos, "Phase behavior of rigid, amphiphilic star polymers," *Soft Matter*, **9**: 7424-7436 (2013). DOI: 10.1039/c3sm51135a *[11]*
204. N. A. Mahynski and A. Z. Panagiotopoulos, "Phase behavior of athermal colloid - star polymer mixtures," *J. Chem. Phys.,* **139:** 024907, 7 pp (2013). 10.1063/1.4811393 *[14]*
205. A. Nikoubashman, R. A. Register, and A. Z. Panagiotopoulos, "Self-Assembly of Cylinder-Forming Diblock Copolymer Thin Films," *Macromolecules*, **46**: 6651-6658 (2013). DOI: 10.1021/ma400867s *[29]*
206. S. Storm, S. Jakobtorweihen, I. Smirnova, and A. Z. Panagiotopoulos, "Molecular Dynamics Simulation of SDS and CTAB Micellization and Prediction of Partition Equilibria with COSMOmic," *Langmuir*, **29**: 11582-92 (2013). DOI: 10.1021/la402415b *[59]*
207. A Nikoubashman, R. A. Register, and A. Z. Panagiotopoulos, "Simulations of shear-induced morphological transitions in block copolymers," *Soft Matter*, **9**: 9960-71 (2013). DOI: 10.1039/c3sm51759d *[35]*

208. K. B. Daly, J. B. Benziger, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Molecular Dynamics Simulations of Water Sorption in a Perfluorosulfonic Acid Membrane," *J. Phys. Chem. B*, **117**: 12649-60 (2013). DOI: 10.1021/jp405440r *[40]*

209. B. Hong and A. Z. Panagiotopoulos, "Atomistic simulation of CO_2 solubility in poly(ethylene oxide) oligomers," *Molec. Phys.*, **112**: 1540-7 (2014). DOI: 10.1080/00268976.2013.842660 *[3]*

210. T. Lafitte, S. K. Kumar, and A. Z. Panagiotopoulos, "Self-Assembly of Polymer-Grafted Nanoparticles in Thin Films," *Soft Matter*, **10**: 786-94 (2014). DOI: 10.1039/c3sm52328d *[81]*

211. A. Chremos, A. Nikoubashman, and A. Z. Panagiotopoulos, "Flory-Huggins parameter χ, from binary mixtures of Lennard-Jones particles to block copolymer melts," *J. Chem. Phys.,* **140**: 054909, 10 pp (2014). DOI: 10.1063/1.4863331 *[91]*

212. A. Nikoubashman, N. A. Mahynski, and A. Z. Panagiotopoulos, "Flow-induced demixing of polymer-colloid mixtures in microfluidic channels," *J. Chem. Phys.,* **140**: 094903, 8 pp (2014); Erratum: in **141**: 149906, 3 pp (2014). DOI: 10.1063/1.4866762 *[20]*

213. A. Nikoubashman, R. A. Register, and A. Z. Panagiotopoulos, "Sequential Domain Realignment Driven by Conformational Asymmetry in Block Copolymer Thin Films," *Macromolecules*, **47**: 1193-8 (2014). DOI: 10.1021/ma402526q *[21]*

214. O. A. Moultos, I. N. Tsimpanogiannis, A. Z. Panagiotopoulos, and I. G. Economou, "Atomistic Molecular Dynamics Simulations of CO_2 Diffusivity in H_2O for a Wide Range of Temperatures and Pressures," *J. Phys. Chem. B* **118**: 5532-41 (2014). DOI: 10.1021/jp502380r *[82]*

215. J. C. Palmer, F. Martelli, Y. Liu, R. Car, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Metastable Liquid–Liquid transition in a Molecular Model of Water," *Nature*, **510**: 385-388 (2014). DOI: 10.1038/nature13405 *[449]*

216. N. A. Mahynski, A. Z. Panagiotopoulos, D. Meng, and S. K. Kumar, "Stabilizing Colloidal Crystals by Leveraging Void Distributions," *Nature Comm.* **5**: 4472, 8 pp (2014). DOI: 10.1038/ncomms5472 *[58]*

217. K. B. Daly, J. B. Benziger, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Molecular Dynamics Simulations of Water Permeation across Nafion Membrane Interfaces," *J. Phys. Chem. B* **118**: 8798-8807 (2014). DOI: 10.1021/jp5024718 *[32]*

218. A. Nikoubashman, R. L. Davis, B. T. Michal, P. M. Chaikin, R. A. Register, and A. Z. Panagiotopoulos, "Thin Films of Homopolymers and Cylinder-Forming Diblock Copolymers under Shear," *ACS Nano*, **8**: 8015-26 (2014). DOI: 10.1021/nn502068e *[34]*

219. A. Nikoubashman and A. Z. Panagiotopoulos, "Effect of solvophobic block length on critical micelle concentration in model surfactant systems," *J. Chem. Phys.* **141**: 041101, 4 pp (2014). DOI: 10.1063/1.4890981 *[5]*

220. J. R. Vella, F. H. Stillinger, A. Z. Panagiotopoulos, and P. G. Debenedetti, "A Comparison of the Predictive Capabilities of Embedded-Atom Method (EAM) and Modified Embedded-Atom Method (MEAM) Potentials for Lithium," *J. Phys. Chem. B* **119**: 8960-8 (2015). DOI: 10.1021/jp5077752 *[25]*

221. G. A. Orozco, I. G. Economou, and A. Z. Panagiotopoulos, "Optimization of Intermolecular Potential Parameters for the CO_2/H_2O Mixture," *J. Phys. Chem. B* **118**: 11504–11 (2014). DOI: 10.1021/jp5067023 *[37]*

222. A. Jusufi and A. Z. Panagiotopoulos, "Explicit- and Implicit-Solvent Simulations of Micellization in Surfactant Solutions," Invited Feature Article, *Langmuir* **31**: 3283-92 (2015). DOI: 10.1021/la502227v *[30]*

223. K. B. Daly, A. Z. Panagiotopoulos, P. G. Debenedetti, and J. B. Benziger, "Viscosity of Nafion oligomers as a function of hydration and counterion type: a molecular dynamics study," *J. Phys. Chem. B* **118**:13981–91 (2014). DOI: 10.1021/jp509061z *[12]*
224. G. A. Orozco, O. A. Moultos, H. Jiang, I. G. Economou, and A. Z. Panagiotopoulos "Molecular Simulation of Thermodynamic and Transport Properties for the H2O + NaCl System," *J. Chem. Phys.*, **141:** 234507, 8 pp (2014). DOI: 10.1063/1.4903928 *[66]*
225. N. A. Mahynski, S. K. Kumar, and A. Z. Panagiotopoulos, "Relative stability of the FCC and HCP polymorphs with interacting polymers," *Soft Matter* **11**: 280 - 289 (2015). DOI: 10.1039/c4sm02191f *[25]*
226. Z. Mester and A. Z. Panagiotopoulos, "Mean ionic activity coefficients in aqueous NaCl solutions from molecular dynamics simulations," *J. Chem. Phys.* **142**: 044507, 10 pp (2015). DOI: 10.1063/1.4906320 *[126]*
227. N. A. Mahynski and A. Z. Panagiotopoulos, "Grafted Nanoparticles as Soft Patchy Colloids: Self-Assembly versus Phase Separation," *J. Chem. Phys.* **142**: 074901, 7 pp (2015). DOI: 10.1063/1.4908044 *[23]*
228. H. Chen, A. Z. Panagiotopoulos, and E. P. Giannelis, "Atomistic Molecular Dynamics Simulations of Carbohydrate-Calcite Interactions in Concentrated Brine," *Langmuir*, **31**: 2407-13 (2015). DOI: 10.1021/la504595g *[52]*
229. O. A. Moultos, G. A. Orozco, I. N. Tsimpanogiannis, Z. A. Makrodimitri, A. Z. Panagiotopoulos, and I. G. Economou, "Atomistic Molecular Dynamics Simulations of H_2O Diffusivity in Liquid and Supercritical CO_2," *Molec. Phys.* **113**: 2805-14 (2015) and Erratum, **113**: 3383 (2015). DOI: 10.1080/00268976.2015.1023224 *[33]*
230. A. Nikoubashman, E. Bianchi, and A. Z. Panagiotopoulos, "Self Assembly of Janus Particles under Shear," *Soft Matter*, **11**: 3767-71 (2015). DOI: 10.1039/c5sm00281h *[47]*
231. C. Koch, A. Z. Panagiotopoulos, F. Lo Verso, and C. N. Likos, "Customizing wormlike mesoscale structures via self-assembly of amphiphilic star polymers," *Soft Matter* **11**: 3530-35 (2015). DOI: 10.1039/c5sm00219b *[19]*
232. O. A. Moultos, I. N. Tsimpanogiannis, A. Z. Panagiotopoulos, and I. G. Economou, "Self-Diffusion Coefficients of the Binary H_2O - CO_2 Mixture at High Temperatures and Pressures," *J. Chem. Thermodyn.*, **93**: 424-429 (2015). DOI: 10.1016/j.jct.2015.04.007 *[45]*
233. M. Chen, J. R. Vella, F. H. Stillinger, E. A. Carter, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Liquid Li Structure and Dynamics: A Comparison Between OFDFT and Second Nearest-Neighbor Embedded-Atom Method," *AIChE J.* **61**: 2841-53 (2015). DOI: 10.1002/aic.14795 *[22]*
234. A. Hemmen, A. Z. Panagiotopoulos, J. Gross, "Grand canonical Monte Carlo simulations guided by an analytic equation of state – Transferable anisotropic Mie-potentials for ethers," *J. Phys. Chem. B* **119**: 7087-99 (2015). DOI: 10.1021/acs.jpcb.5b01806 *[32]*
235. N. A. Mahynski, S. K. Kumar, and A. Z. Panagiotopoulos, "Tuning Polymer Architecture to Manipulate the Relative Stability of Different Colloid Crystal Morphologies," *Soft Matter* **11**: 5146-53 (2015). DOI: 10.1039/C5SM00631g *[13]*
236. E. Tsai, H. Jiang, and A. Z. Panagiotopoulos, "Monte Carlo Simulations of H_2O-$CaCl_2$ and H_2O-$CaCl_2$-CO_2 Mixtures," *Fluid Phase Equil.* **407**: 262-68 (2016). DOI: 10.1016/j.fluid.2015.05.036 *[15]*
237. M. P. Howard, A. Z. Panagiotopoulos and A. Nikoubashman, "Inertial and viscoelastic forces on rigid colloids in microfluidic channels," *J. Chem. Phys.* **142**: 224908, 9 pp (2015). DOI: 10.1063/1.4922323 *[20]*

238. Z. Mester and A. Z. Panagiotopoulos, "Temperature-Dependent Solubilities and Mean Ionic Activity Coefficients of Alkali Halides in Aqueous Solutions from Molecular Dynamics Simulations," *J. Chem. Phys.* **143**: 044505, 10 pp (2015). DOI: 10.1063/1.4926840 *[84]*

239. H. Jiang, Z. Mester, O. A. Moultos, I. G. Economou, and A. Z. Panagiotopoulos, "Thermodynamic and Transport Properties of H_2O+NaCl from Polarizable Force Fields," *J. Chem. Theory Comput.* **11**: 3802-3810 (2015). DOI: 10.1021/acs.jctc.5b00421 *[63]*

240. A. Nikoubashman, N. A. Mahynski, B. Capone, A. Z. Panagiotopoulos, and C. N. Likos, "Coarse graining and phase behavior of model star polymer--colloid mixtures in solvents of varying quality," *J. Chem. Phys.* **143**: 243108 (2015). DOI: 10.1063/1.4931410 *[7]*

241. H. Jiang, A. Z. Panagiotopoulos and I. G. Economou, "Modeling of CO_2 Solubility in Single and Mixed Electrolyte Solutions Using Statistical Associating Fluid Theory," *Geochim. Cosmochim. Acta* **176**: 185-197 (2016). DOI: 10.1016/j.gca.2015.12.023 *[22]*

242. A. Nikoubashman, V. E. Lee, C. Sosa, R. K. Prud'homme, R. D. Priestley, and A. Z. Panagiotopoulos, "Directed assembly of soft colloids through rapid solvent exchange," *ACS Nano* **10**: 1425-33 (2016). DOI: 10.1021/acsnano.5b06890 *[73]*

243. A. P. Santos and A. Z. Panagiotopoulos, "Determination of the critical micelle concentration in simulations of surfactant systems," *J. Chem. Phys.* **144**: 044709, 10 pp (2016). DOI: 10.1063/1.4940687 *[56]*

244. H. Jiang, O. A. Moultos, I. G. Economou, and A. Z. Panagiotopoulos, "Gaussian-Charge Polarizable and Non-Polarizable Models for CO_2," *J. Phys. Chem. B* **120**: 984-994 (2016). DOI: 10.1021/acs.jpcb.5b11701 *[32]*

245. J. C. Palmer, F. Martelli, Y. Liu, R. Car, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Metastability and no criticality: reply," *Nature* **531**: E2-E3 (2016). DOI: 10.1038/nature16540 *[14]*

246. M. P. Howard, J. A. Anderson, A. Nikoubashman, S. C. Glotzer, and A. Z. Panagiotopoulos, "Efficient neighbor list calculation for molecular simulation of colloidal systems using graphics processing units," *Comp. Phys. Comm*. **203**: 45-52 (2016). DOI: 10.1016/j.cpc.2016.02.003 *[57]*

247. N. A. Mahynski, L. Rovigatti, C. N. Likos, and A. Z. Panagiotopoulos, "Bottom-Up Colloidal Crystal Assembly with a Twist," *ACS Nano* **10**: 5459-67 (2016). DOI: 10.1021/acsnano.6b01854 *[30]*

248. H. Chen, J. R. Cox, and A. Z Panagiotopoulos, "Force Fields for Carbohydrate-Divalent Cation Interactions," *J. Phys. Chem. B* **120**: 5203-8 (2016). DOI: 10.1021/acs.jpcb.6b01438 *[9]*

249. P. Gallo, K. Amann-Winkel, C. A. Angell, M. A. Anisimov, F. Caupin, C. Chakravarty, E. Lascaris, T. Loerting, A. Z. Panagiotopoulos, J. Russo, J. A. Sellberg, H. E. Stanley, H. Tanaka, C. Vega, L. Xu, and L. G. M. Pettersson, "Water: A Tale of Two Liquids," *Chem. Rev.* **116**: 7463-7500 (2016). DOI: 10.1021/acs.chemrev.5b00750 *[653]*

250. H. Chen, J. R. Cox, H. Ow, R. Shi, and A. Z Panagiotopoulos, "Hydration Repulsion between Carbohydrate Surfaces Mediated by Temperature and Specific Ions," *Scientific Reports* **6**: 28553, 10 pp (2016). DOI: 10.1038/srep28553 *[19]*

251. H. Jiang and A. Z. Panagiotopoulos, "Activity coefficients and solubilities for the NaCl/ϵ force field," *J. Chem. Phys.* **145:** 046101, 2 pp (2016). DOI: 10.1063/1.4959789 *[11]*

252. M. P. Howard, A. Gautam, A. Z. Panagiotopoulos, and A. Nikoubashman, "Axial dispersion of Brownian colloids in microfluidic channels," *Phys. Rev. Fluids* **1**: 044203, 20 pp (2016). DOI: 10.1103/PhysRevFluids.1.044203 *[16]*

253. W. F. Reinhart and A. Z. Panagiotopoulos, "Equilibrium crystal phases of triblock Janus colloids," *J. Chem. Phys.* **145**: 094505, 11 pp (2016). DOI: 10.1063/1.4961869 *[35]*

254. J. R. Espinosa, J. M. Young, H. Jiang, D. Gupta, C. Vega, E. Sanz, P. G. Debenedetti, and A. Z. Panagiotopoulos, "On the calculation of solubilities via direct coexistence simulations: Investigation of NaCl aqueous solutions and Lennard-Jones binary mixtures," *J. Chem. Phys.,* **145**: 154111, 7 pp (2016). DOI: 10.1063/1.4964725 *[89]*

255. O. A. Moultos, I. N. Tsimpanogiannis, A. Z. Panagiotopoulos, J. P. M. Trusler, I. G. Economou, "Atomistic Molecular Dynamics Simulations of Carbon Dioxide Diffusivity in n-Hexane, n-Decane, n-Hexadecane, Cyclohexane and Squalane," *J. Phys. Chem. B*, **120**: 12890-12900 (2016). DOI: 10.1021/acs.jpcb.6b04651 *[59]*

256. H. Jiang, O. A. Moultos, I. G. Economou, A. Z. Panagiotopoulos, "A Hydrogen-Bonding Polarizable Intermolecular Potential Model for Water," *J. Phys. Chem. B*, **120**: 12358-70 (2016). DOI: 10.1021/acs.jpcb.6b08205 *[44]*

257. K. S. Silmore, M. P. Howard, A. Z. Panagiotopoulos, "Vapour–liquid phase equilibrium and surface tension of fully flexible Lennard–Jones chains," *Molec. Phys.* **115**: 320-327 (2017). DOI: 10.1080/ 00268976.2016.1262075 *[66]*

258. J. R. Vella, M. Chen, F. H. Stillinger, E. A. Carter, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Structural and dynamic properties of liquid tin from a new modified embedded-atom method force field," *Phys. Rev. B*, **95**: 064202 (2017). DOI: 10.1103/PhysRevB.95.064202 *[24]*

259. D. Meng, S. K. Kumar, G. S. Grest, N. A. Mahynski, and A. Z. Panagiotopoulos, "Reentrant equilibrium disordering in nanoparticle–polymer mixtures," *NPJ Comput. Mater.*, **3**: 3 (2017). DOI: 10.1038/s41524-016-0005-8 *[4]*

260. H. Jiang, I. G. Economou, and A. Z. Panagiotopoulos, "Phase Equilibria of Water/CO_2 and Water/n-Alkane Mixtures from Polarizable Models," *J. Phys. Chem. B*, **121**: 1386-95 (2017). DOI: 10.1021/acs.jpcb.6b12791 *[31]*

261. H. Jiang, I. G. Economou, and A. Z. Panagiotopoulos, "Molecular Modeling of Thermodynamic and Transport Properties for CO_2 and Aqueous Brines," *Acc. Chem. Res.*, **50**: 751-8 (2017). DOI: 10.1021/acs.accounts.6b00632 *[29]*

262. N. Li, A. Z. Panagiotopoulos, and A. Nikoubashman, "Structured nanoparticles from the self-assembly of polymer blends through rapid solvent exchange," *Langmuir*, **33**: 6021- 8 (2017). DOI: 10.1021/acs.langmuir.7b00291 *[33]*

263. M. P. Howard, A. Nikoubashman, and A. Z. Panagiotopoulos, "Stratification dynamics in drying colloidal mixtures," *Langmuir*, **33**: 3685-93 (2017). DOI: 10.1021/acs...7b00543 *[88]*

264. W. Liu, N. A. Mahynski, O. Gang, A. Z. Panagiotopoulos, and S. K. Kumar, "Directionally Interacting Spheres and Rods Form Ordered Phases," *ACS Nano*, **11**: 4950-9 (2017). DOI: 10.1021/acsnano.7b01592 *[16]*

265. W. F. Reinhart, A. W. Long, M. P. Howard, A. L. Ferguson and A. Z. Panagiotopoulos, "Machine learning for autonomous crystal structure identification," *Soft Matter,* **13**: 4733-45 (2017). DOI: 10.1039/c7sm00957g *[98]*

266. M. P. Howard, A. Statt and A. Z. Panagiotopoulos, "Note: Smooth torsional potentials for degenerate dihedral angles," *J. Chem. Phys.,* **146**: 226101 (2017); Erratum in **154**: 099901 (2021) DOIs: 10.1063/1.4985251and 10.1063/5.0046594 *[8]*

267. J. R. Vella, M. Chen, S. Fürstenberg, F. H. Stillinger, E. A. Carter, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Characterization of the liquid Li-solid Mo (110) interface from

classical molecular dynamics for plasma-facing applications," *Nucl. Fusion*, **57**: 116036 (2017). DOI: 10.1088/1741-4326/aa7e0d *[9]*

268. M. P. Howard, A. Nikoubashman and A. Z. Panagiotopoulos, "Stratification in drying polymer-polymer and colloid-polymer mixtures," *Langmuir*, **33**: 11390-98 (2017). DOI: 10.1021/acs.langmuir.7b02074 *[60]*
269. W. F. Reinhart and A. Z. Panagiotopoulos, "Multi-atom pattern analysis for binary superlattices," *Soft Matter*, **13**: 6803-9 (2017). DOI: 10.1039/c7sm01642e *[16]*
270. H. Jiang, F. Müller-Plathe and A. Z. Panagiotopoulos, "Contact angles from Young's equation in molecular dynamics simulations," *J. Chem. Phys.*, **147**: 084708 (2017). DOI: 10.1063/1.4994088 *[56]*
271. A. P. Santos, J. Pękalski, and A. Z. Panagiotopoulos, "Thermodynamic signatures and cluster properties of self-assembly in systems with competing interactions," *Soft Matter*, **13**: 8055-63 (2017). DOI: 10.1039/c7sm01721a *[31]*
272. A. Statt, M. P. Howard, and A. Z. Panagiotopoulos, "Solvent quality influences surface structure of glassy polymer thin films after evaporation," *J. Chem. Phys.* **147**: 184901 (2017). DOI: 10.1063/1.4996119 *[12]*
273. J. Schneider, A. Z. Panagiotopoulos, and F. Müller-Plathe, "Polymer Chain Collapse Upon Rapid Solvent Exchange: Slip-Spring Dissipative-Particle-Dynamics Simulations with an Explicit-Solvent Model," *J. Phys. Chem. C,* **121**: 27664-73 (2017) DOI: 10.1021/acs.jpcc.7b07135 *[10]*
274. N. Li, A. Nikoubashman, and A. Z. Panagiotopoulos, "Controlled production of patchy particles from the combined effects of nanoprecipitation and vitrification," *Soft Matter*, **13**: 8433- 41 (2017). DOI: 10.1039/C7SM01896G *[15]*
275. S. Jiao, A. P. Santos, and A. Z. Panagiotopoulos, "Differences in free surfactant concentration and aggregation properties for amphiphiles with the same critical micelle concentration," *Fluid Phase Equil.*, **470**: 126-33 (2018). DOI: 10.1016/j.fluid.2017.10.026 *[14]*
276. J. M. Young and A. Z. Panagiotopoulos, "System-size dependence of electrolyte activity coefficients in molecular simulations," *J. Phys. Chem. B*, **122**: 3330-8 (2018). DOI: 10.1021/acs.jpcb.7b09861 *[21]*
277. H. Chen, and A. Z. Panagiotopoulos, "Communication: Modeling electrolyte mixtures with concentration dependent dielectric permittivity," *J. Chem. Phys.*, **148**: 041102 (2018). DOI: 10.1063/1.5018195 *[9]*
278. H. Jiang, A. Haji-Akbari, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Forward flux sampling calculation of homogeneous nucleation rates from aqueous NaCl solutions," *J. Chem. Phys.*, **148**: 044505 (2018). DOI: 10.1063/1.5016554 *[54]*
279. W. F. Reinhart and A. Z. Panagiotopoulos, "Crystal growth kinetics of triblock Janus colloids," *J. Chem. Phys.*, **148**: 124506 (2018). DOI: 10.1063/1.5021347 *[16]*
280. J. C. Palmer, A. Haji-Akbari, R. S. Singh, F. Martelli, R. Car, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Comment on "The putative liquid-liquid transition is a liquid-solid transition in atomistic models of water" [I and II: J. Chem. Phys. 135, 134503 (2011); J. Chem. Phys. 138, 214504 (2013)]," *J. Chem. Phys.,* **148**: 137101 (2018). DOI: 10.1063/1.5029463 *[51]*
281. M. P. Howard, A. Z. Panagiotopoulos, and A. Nikoubashman, "Efficient mesoscale hydrodynamics: Multiparticle collision dynamics with massively parallel GPU acceleration," *Comp. Phys. Commun*. **230**: 10-20 (2018). DOI: 10.1016/j.cpc.2018.04.009 *[42]*

282. L. S. Grundy, V. E. Lee, N. Li, C. Sosa, W. D. Mulhearn, R. Liu, R. A. Register, A. Nikoubashman, R. K. Prud'homme, A. Z. Panagiotopoulos, and R. D. Priestley, "Rapid Production of Internally Structured Colloids by Flash NanoPrecipitation of Block Copolymer Blends," *ACS Nano* **12**: 4660-8 (2018). DOI: 10.1021/acsnano.8b01260 *[80]*

283. A. Statt, M. P. Howard, and A. Z. Panagiotopoulos, "Influence of hydrodynamic interactions on stratification in drying mixtures," *J. Chem. Phys.*, **149**: 024902 (2018). DOI: 10.1063/1.5031789 *[29]*

284. W. F. Reinhart and A. Z. Panagiotopoulos "Automated crystal characterization with a fast Neighborhood Graph Analysis method," *Soft Matter* **14**: 6083-9 (2018). DOI: 10.1039/c8sm00960k *[35]*

285. N. Li, A. Nikoubashman, and A. Z. Panagiotopoulos, "Multi-scale simulations of polymeric nanoparticle aggregation during rapid solvent exchange," *J. Chem. Phys.*, **149**: 084904 (2018). (Editor's Choice) DOI: 10.1063/1.5046159 *[13]*

286. M. P. Howard, W. F. Reinhart, T. Sanyal, M. S. Shell, A. Nikoubashman, and A. Z. Panagiotopoulos, "Evaporation-induced assembly of colloidal crystals," *J. Chem. Phys.*, **149**: 094901 (2018); Erratum **149**: 209902 (2018). DOI: 10.1063/1.5043401 *[36]*

287. H. Jiang, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Communication: Nucleation rates of supersaturated aqueous NaCl using a polarizable force field," *J. Chem. Phys.*, **149**: 141102 (2018). DOI: 10.1063/1.5053652 *[17]*

288. W. F. Reinhart and A. Z. Panagiotopoulos "Directed assembly of photonic crystals through simple substrate patterning," *J. Chem. Phys.* **150**: 014503 (2019). DOI: 10.1063/1.5070153 *[5]*

289. T. I. Morozova, V. E. Lee, A. Z. Panagiotopoulos, R. K. Prud'homme, R. D. Priestley, and A. Nikoubashman, "On the Stability of Polymeric Nanoparticles Fabricated through Rapid Solvent Mixing," *Langmuir*, **35**: 709-17 (2019). DOI: 10.1021/acs.langmuir.8b03399 *[26]*

290. H. Chen and A. Z. Panagiotopoulos, "Molecular Modeling of Surfactant Micellization Using Solvent Accessible Surface Area," *Langmuir*, **35**: 2443-50 (2019). DOI: 10.1021/acs.langmuir.8b03440 *[39]*

291. N. Li, A. Nikoubashman, and A. Z. Panagiotopoulos, "Self-assembly of polymer blends and nanoparticles through rapid solvent exchange," *Langmuir*, **35**: 3780-9 (2019). DOI: 10.1021/acs.langmuir.8b04197 *[8]*

292. H. Jiang, P. G. Debenedetti, and A. Z. Panagiotopoulos, "Nucleation in aqueous NaCl solutions shifts from 1-step to 2-step mechanism on crossing the spinodal," *J. Chem. Phys.*, **150**: 124502 (2019). [Cover article] DOI: 10.1063/1.5084248 *[76]*

293. M. P. Howard, A. Statt, F. Madutsa, T. M. Truskett, and A. Z. Panagiotopoulos, "Quantized bounding volume hierarchies for neighbor search in molecular simulations on graphics processing units," *Comp. Mat. Sci.*, **164**: 139-146 (2019). DOI: 10.1016/...2019.04.004 *[12]*

294. A. Statt, M. P. Howard, and A. Z. Panagiotopoulos, "Unexpected secondary flows in reverse nonequilibrium shear flow simulations," *Phys. Rev. Fluids*, **4**:043905 (2019). DOI: 10.1103/PhysRevFluids.4.043905 *[9]*

295. R. S. Singh, J. C. Palmer, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Thermodynamic analysis of the stability of planar interfaces between coexisting phases and its application to supercooled water," *J. Chem. Phys.,* **150**: 224503 (2019). DOI: 10.1063/1.5097591 *[12]*

296. E. Moghimi, I. Chubak, A. Statt, M. P. Howard, D. Founta, G. Polymeropoulos, K. Ntetsikas, N. Hadjichristidis, A. Z. Panagiotopoulos, C. N. Likos, and D. Vlassopoulos, "Self-Organization and Flow of Low-Functionality Telechelic Star Polymers with Varying Attraction," *ACS Macro Lett.*, **8**: 766-772 (2019). DOI: 10.1021/acsmacrolett.9b00211 *[13]*

297. S. Yue and A. Z. Panagiotopoulos, "Dynamic properties of aqueous electrolyte solutions from non-polarisable, polarisable, and scaled-charge models," *Molec. Phys.*, **117**: 3538-49 (2019). DOI: 10.1080/00268976.2019.1645901 *[34]*

298. J. M. Young, C. Tietz, and A. Z. Panagiotopoulos, "Activity Coefficients and Solubility of $CaCl_2$ from Molecular Simulations," *J. Chem. Eng. Data*, **65**: 337-48 (2020). DOI: 10.1021/acs.jced.9b00688 *[16]*

299. A. Statt, H. Casademunt, C. P. Brangwynne, and A. Z. Panagiotopoulos, "Model for disordered proteins with strongly sequence-dependent liquid phase behavior," *J. Chem. Phys.,* **152**: 075101 (2020). DOI: 10.1063/1.5141095 *[116]*

300. J. Pękalski, W. Rządkowski, and A. Z. Panagiotopoulos, "Shear induced ordering in systems with competing interactions: A machine learning study," *J. Chem. Phys.,* **152**: 204905 (2020). DOI: 10.1063/5.0005194 *[8]*

301. A. Z. Panagiotopoulos, "Simulations of activities, solubilities, transport properties, and nucleation rates for aqueous electrolyte solutions," *J. Chem. Phys.,* **153**: 010903 (2020) [Featured Article]. DOI: 10.1063/5.0012102 *[42]*

302. D. Kussainova, A. Mondal, J. M. Young, S. Yue, and A. Z. Panagiotopoulos, "Molecular simulation of liquid–vapor coexistence for NaCl: Full-charge vs scaled-charge interaction models," *J. Chem. Phys.,* **153**: 024501 (2020). DOI: 10.1063/5.0012065 *[11]*

303. A. Mondal, J. M. Young, T. A. Barckholtz, G. Kiss, L. Koziol, and A. Z. Panagiotopoulos, "Genetic Algorithm Driven Force Field Parameterization for Molten Alkali-Metal Carbonate and Hydroxide Salts," *J. Chem. Theory Comput.*, **16**: 5736-46 (2020). DOI: 10.1021/ acs.jctc.0c00285 *[14]*

304. J. M. Young, A. Mondal, T. A. Barckholtz, G. Kiss, L. Koziol, and A. Z. Panagiotopoulos, "Predicting chemical reaction equilibria in molten carbonate fuel cells via molecular simulations," *AIChE J.*, **67**: e16988 (2021). DOI: 10.1002/aic.16988 *[9]*

305. A. Mondal, J. M. Young, T. A. Barckholtz, G. Kiss, L. Koziol, and A. Z. Panagiotopoulos, "Transport and Interfacial Properties of Mixed Molten Carbonate/Hydroxide Electrolytes by Molecular Dynamics Simulations," *J. Phys. Chem. C*, **124**: 23532-40 (2020). DOI: 10.1021/acs.jpcc.0c07295 *[7]*

306. T. E. Gartner III, L. Zhang, P. M. Piaggi, R. Car, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Signatures of a liquid–liquid transition in an ab initio deep neural network model for water," *Proc. Natl. Acad. Sci.*, **117**: 26040-6 (2020). DOI: 10.1073/pnas.2015440117 *[129]*

307. S. Yue, M. C. Muniz, M. F. C. Andrade, L. Zhang, R. Car, and A. Z. Panagiotopoulos, "When do short-range atomistic machine learning models fall short?" *J. Chem. Phys*. **154**: 034111 (2021). [Selected as Featured Article] DOI: 10.1063/5.0031215 *[77]*

308. A. Mondal, J. M. Young, G. Kiss, and A. Z. Panagiotopoulos, "First-Principles Modeling of Transport Mechanisms in Carbonate–Hydroxide Electrolytes," *J. Phys. Chem. C*, **125**: 4412-22 (2021). DOI: 10.1021/acs.jpcc.0c10879 *[4]*

309. P. M. Piaggi, A. Z. Panagiotopoulos, P. G. Debenedetti, and R. Car, "Phase Equilibrium of Water with Hexagonal and Cubic Ice Using the SCAN Functional," *J. Chem. Theory Comput.* **17**: 3065-77 (2021). DOI: 10.1021/acs.jctc.1c00041 *[47]*

310. M. C. Muniz, T. E. Gartner, M. Riera, C. Knight, S. Yue, F. Paesani, and A. Z. Panagiotopoulos, "Vapor-liquid equilibrium of water with the MB-pol many-body potential," *J. Chem. Phys.*, **154**: 211103 (2021). [Editor's pick] DOI: 10.1063/5.0050068 *[40]*

311. S. H. Saravi and A. Z. Panagiotopoulos, "Individual Ion Activity Coefficients in Aqueous Electrolytes from Explicit-Water Molecular Dynamics Simulations," *J. Phys. Chem. B*, **125**: 8511-21 (2021). DOI: 10.1021/acs.jpcb.1c04019 *[22]*
312. U. Rana, C. P. Brangwynne, and A. Z. Panagiotopoulos, "Phase separation versus aggregation behavior for model disordered proteins," *J. Chem. Phys.*, **155**: 125101 (2021). [Cover article / Editor's pick] DOI: 10.1063/5.0060046 *[42]*
313. S. H. Saravi and A. Z. Panagiotopoulos, "Activity coefficients of aqueous electrolytes from implicit-water molecular dynamics simulations," *J. Chem. Phys.*, **155**: 184501 (2021). DOI: 10.1063/5.0064963 *[9]*
314. C. Zhang, S. Yue, A. Z. Panagiotopoulos, M. L. Klein, and X. Wu, "Dissolving salt is not equivalent to applying a pressure on water," *Nature Commun.*, **13**: 822 (2022). DOI: 10.1038/s41467-022-28538-8 *[56 + 2]*
315. S. Yue, M. Riera, R. Ghosh, A. Z. Panagiotopoulos, and F. Paesani, "Transferability of data-driven, many-body models for CO_2 simulations in the vapor and liquid phases," *J. Chem. Phys.*, **156**: 104503 (2022). DOI: 10.1063/5.0080061 *[14]*
316. L. Zhang, H. Wang, M. C. Muniz, A. Z. Panagiotopoulos, R. Car, and W. E, "A deep potential model with long-range electrostatic interactions," *J. Chem. Phys.*, **156**: 124107 (2022). [Editor's pick] DOI: 10.1063/5.0083669 *[76]*
317. S. H. Saravi and A. Z. Panagiotopoulos, "Activity Coefficients and Solubilities of NaCl in Water–Methanol Solutions from Molecular Dynamics Simulations," *J. Phys. Chem. B*, **126**: 2891-8 (2022). DOI: 10.1021/acs.jpcb.2c00813 *[7]*
318. T. E. Gartner III., K. M. Hunter, E. Lambros, A. Caruso, M. Riera, G. R. Medders, A. Z. Panagiotopoulos, P. G. Debenedetti, F. Paesani, "Anomalies and Local Structure of Liquid Water from Boiling to the Supercooled Regime as Predicted by the Many-Body MB-pol Model," *J. Phys. Chem. Lett.* **13**: 3652-3658 (2022). DOI: 10.1021/acs.jpclett.2c00567 *[40]*
319. J. Weis, F. Sciortino, A. Z. Panagiotopoulos, and P. G. Debenedetti, "Liquid-Liquid Criticality in the WAIL Water Model," *J. Chem. Phys.*, **157**: 124107 (2022). DOI: 10.1063/5.0099520 *[24]*
320. P. M. Piaggi, J. Weis, A. Z. Panagiotopoulos, P. G. Debenedetti, and R. Car, "Homogeneous ice nucleation in an ab initio machine-learning model of water," *Proc. Natl. Acad. Sci.*, **119:** e2207294119 (2022). DOI: 10.1073/pnas.2207294119 *[44]*
321. T. E. Gartner, P. M. Piaggi, R. Car, A. Z. Panagiotopoulos and P. G. Debenedetti, "Liquid-Liquid Transition in Water from First Principles," *Phys. Rev. Lett.*, **129**: 255702 (2022). DOI: 10.1103/PhysRevLett.129.255702 *[35]*
322. A. Mondal, D. Kussainova, S. Yue, and A. Z. Panagiotopoulos, "Modeling Chemical Reactions in Alkali Carbonate−Hydroxide Electrolytes with Deep Learning Potentials," *J. Chem. Theory Comput.* **19:** 4584-95 (2023). DOI: 10.1021/acs.jctc.2c00816 *[12]*
323. A. Z. Panagiotopoulos and S. Yue, "Dynamics of Aqueous Electrolyte Solutions: Challenges for Simulations," *J. Phys. Chem. B* **127**: 430-37 (2023). DOI: 10.1021/acs.jpcb.2c07477 *[13]*
324. A. Z. Panagiotopoulos, "Phase Separation and Aggregation in Multiblock Chains," *J. Chem. Phys.* **158**: 154901 (2023). [Editor's pick] DOI: 10.1063/5.0146673 *[4]*
325. I. Sanchez-Burgos, M. C. Muniz, J. R. Espinosa, and A. Z. Panagiotopoulos, "A Deep Potential Model for Liquid-vapor Equilibrium and Cavitation Rates of Water," *J. Chem. Phys.* **158**: 184504 (2023). [Scilight] DOI: 10.1063/5.0144500 *[12]*

326. R. Mathur, M. C. Muniz, S. Yue, R. Car, and A. Z. Panagiotopoulos, "First-Principles-Based Machine Learning Models for Phase Behavior and Transport Properties of CO_2", *J. Phys. Chem. B* **127**: 4562-69 (2023). DOI: 10.1021/acs.jpcb.3c00610 *[8]*
327. C. Zhang, S. Yue, A. Z. Panagiotopoulos, M. L. Klein, and X. Wu, "Why dissolving salt in water decreases its dielectric permittivity," *Phys. Rev. Lett.* **131**:076801 (2023). DOI: 10.1103/PhysRevLett.131.076801 *[6]*
328. M. C. Muniz, R. Car, and A. Z. Panagiotopoulos, "Neural network water model based on the MB-Pol many-body potential," *J. Phys. Chem. B* **127**: 9165-71 (2023). DOI: 10.1021/acs.jpcb.3c04629 *[7]*
329. P. M. Piaggi, A. Selloni, A. Z. Panagiotopoulos, R. Car, and P. G. Debenedetti, "A first-principles machine-learning force field for heterogeneous ice nucleation on microcline feldspar," *Faraday Trans.* **249**: 98-113 (2024). DOI: 10.1039/d3fd00100h *[10]*
330. D. Kussainova and A. Z. Panagiotopoulos, "Molecular Simulation of Lithium Carbonate Reactive Vapor-Liquid Equilibria using a Deep Potential Model," *J. Chem. Eng. Data* **69**: 204-214 (2024). DOI: 10.1021/acs.jced.3c00580
331. E. Moghimi, I. Chubak, K. Ntetsikas, G. Polymeropoulos, X. Wang, C. Carillo, A. Statt, L. Cipelletti, K. Mortensen, N. Hadjichristidis, A. Z. Panagiotopoulos, C. N. Likos, and D. Vlassopoulos, "Interpenetrated and Bridged Nanocylinders from Self-Assembled Star Block Copolymers," *Macromolecules* **57**: 926-39 (2024). DOI: 10.1021/acs.macro...02088
332. U. Rana, K. Xu, A. Narayanan, M. T. Walls, A. Z. Panagiotopoulos, J. L. Avalos, and C. P. Brangwynne, "Asymmetric oligomerization state and sequence patterning can tune multiphase condensate miscibility," *Nature Chem.* (2024). DOI: 10.1038/s41557-024-01456-6 *[9+4]*
334. U. Rana, N. S. Wingreen, C. P. Brangwynne, and A. Z. Panagiotopoulos, "Interfacial exchange dynamics of biomolecular condensates are highly sensitive to client interactions," *J. Chem. Phys.* **160**: 145102 (2024). DOI: 10.1063/5.0188461 *[2]*
335. A. Z. Panagiotopoulos, "Sequence dependence of critical properties for two-letter chains," *J. Chem. Phys.* **160:** 234902 (2024). [Editor's pick] DOI: 10.1063/5.0215700 *[1]*
336. A. Z. Panagiotopoulos, "Solvent Selectivity controls Micro- versus Macrophase Separation in Multiblock Chains," *Macromolecules* **57:** 8253-61 (2024). DOI: 10.1021/acs.macromol.4c01214 *[]*
337. J. S. Draney, J. R. Vella, A. Z. Panagiotopoulos, and D. B. Graves, "Atomic Scale Etching of Diamond: Insights from Molecular Dynamics Simulations," *J. Phys. D*: *Appl. Phys.* **XX:** xx (2024). DOI: 10.1088/1361-6463/ad78e6
338. D. Kussainova and A. Z. Panagiotopoulos, "Simulation of Lithium Hydroxide Decomposition using Deep Potential Molecular Dynamics," *J. Chem. Phys.* **XX**: xx (2024). DOI: 10.1063/