

**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)

*POSITIONS SINCE FIRST DEGREE*

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-present)

*SELECTED HONORS*

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  
American Academy of Arts and Sciences, 2012  
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*

*Molecular Physics*, Editorial Board, 1998 – 2007, Advisory Board, 2008 – present  
*AIChE J.*, Consulting Editors Board, 2012 – present  
*J. Chem. Eng. Data*, Editorial Advisory Board, 2016 – present

*BOOK*

*Essential Thermodynamics*, Drios Press, 2011 (undergraduate textbook)

## REFEREED PUBLICATIONS

Citation data as of Aug. 28, 2020: [Google Scholar](#): 21,559 total citations,  $h=73$ ; *Web of Science*: 16,062 total citations,  $h=62$ .

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](#) [193]
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](#) [76]
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](#) [17]
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](#) [64]
6. 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/jc00053a028](#) [23]
7. 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](#) [28]
8. 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](#) [1,662+17]
9. 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](#) [264]
10. 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](#) [122]
11. 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](#) [960]
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](#) [49]
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](#) [96]

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](https://doi.org/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](https://doi.org/10.1016/0378-3812(89)80080-9) [38]
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](https://doi.org/10.1063/1.458138) [63]
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<sub>6</sub>, or refrigerant 13 (CClF<sub>3</sub>), 23 (CF<sub>3</sub>H) or 116 (C<sub>2</sub>F<sub>6</sub>)," *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](https://doi.org/10.1016/0378-3812(91)87014-Z) [80]
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). [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](https://doi.org/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](https://doi.org/10.1103/PhysRevLett.66.2935) [147]
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](https://doi.org/10.1016/0378-3812(92)85080-R) [123]
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: [10.1080/08927029208048258](https://doi.org/10.1080/08927029208048258) [303]
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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1063/1.463383) [62]
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](https://doi.org/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](https://doi.org/10.1016/0378-3812(93)87025-V) [6]
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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](https://doi.org/10.1080/00268979400100481) [147]
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](https://doi.org/10.1007/978-94-015-8295-7_16) [16]
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](https://doi.org/10.1016/0378-3812(94)87049-7) [22]
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](https://doi.org/10.1021/ma00080a012) [104]
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](https://doi.org/10.1016/0009-2509(94)E0110-C) [15]
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](https://doi.org/10.1063/1.467770) [197]
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](https://doi.org/10.1016/0378-3812(94)80007-3) [49]
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](https://doi.org/10.1209/0295-5075/27/7/010) [20]
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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1007/BF01458815) [121]
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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](https://doi.org/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](https://doi.org/10.1007/978-94-011-0065-6_11) [54+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: [10.1063/1.469869](https://doi.org/10.1063/1.469869) [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](https://doi.org/10.1016/0378-3812(95)02894-3) [34]
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](https://doi.org/10.1021/ma951343y) [29]
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](https://doi.org/10.1063/1.471026) [52]
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](https://doi.org/10.1063/1.471406) [34]
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: [10.1080/002689796173426](https://doi.org/10.1080/002689796173426) [43]
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](https://doi.org/10.1063/1.472721) [71]
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](https://doi.org/10.1103/PhysRevLett.77.4386) [112]
56. K. Kiyohara, K. E. Gubbins, and A. Z. Panagiotopoulos, "Phase Coexistence Properties of Polarizable Stockmayer Fluids," *J. Chem. Phys.*, **106**, 3338-47 (1997). DOI: [10.1063/1.473082](https://doi.org/10.1063/1.473082) [48]
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](https://doi.org/10.1021/la961090h) [139]
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](https://doi.org/10.1021/ma971108a) [133]
59. K. Kiyohara, K.E. Gubbins, and A.Z. Panagiotopoulos, "Phase Coexistence Properties of Polarizable Water Models," *Molec. Phys.*, **94**, 803-8 (1998). DOI: [10.1080/002689798167638](https://doi.org/10.1080/002689798167638) [105]
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](https://doi.org/10.1016/S0378-3812(98)00273-8) [22]



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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](https://doi.org/10.1021/jp981627v) [106]
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](https://doi.org/10.1021/jp982068v) [163]
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](https://doi.org/10.1063/1.477687) [60]
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](https://doi.org/10.1063/1.477798) [215]
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](https://doi.org/10.1063/1.477787) [300]
67. M.A. Floriano, E. Caponetti, and A.Z. Panagiotopoulos, "Micellization in Model Surfactant Systems," *Langmuir*, **15**, 3143-3151 (1999). DOI: [10.1021/la9810206](https://doi.org/10.1021/la9810206) [173]
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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](https://doi.org/10.1103/PhysRevLett.82.5060) [57]
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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](https://doi.org/10.1088/0953-8984/12/3/201) [254+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](https://doi.org/10.1103/PhysRevLett.83.2981) [99]
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](https://doi.org/10.1063/1.480308) [110]
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](https://doi.org/10.1063/1.481264) [52]
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