

**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; 2<sup>nd</sup> Ed. 2026 (undergraduate textbook).

**PUBLICATIONS**

Citation data as of Feb. 20, 2026: [Google Scholar](#): 29,655 citations,  $h=86$ ; *Web of Science*: 24,310 citations,  $h=78$ .

1. A. Z. Panagiotopoulos and S. K. Kumar, "A generalized technique to obtain pure component parameters for two-parameter equations of state," *Fluid Phase Equil.* **22**: 77-88 (1985). DOI: [10.1016/0378-3812\(85\)87012-6](#) [*Web of Science citations*: 23]
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](#) [213]
3. A. Z. Panagiotopoulos and R. C. Reid, "Multiphase high-pressure equilibria in ternary aqueous systems," *Fluid Phase Equil.* **29**: 525-534 (1986). DOI: [10.1016/...85051-8](#) [81]
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](#) [71]
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](#) [33]
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](#) [1,975 +32]
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](#) [300]
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](#) [130]
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](#) [1,156]
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](#) [56]
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](https://doi.org/10.1007/BF01133541) [118]
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 Equil.* **53**: 133-141 (1989). DOI: [10.1016/0378-3812\(89\)80080-9](https://doi.org/10.1016/0378-3812(89)80080-9) [41]
  16. K. E. Gubbins and A. Z. Panagiotopoulos, “Molecular Simulation,” *Chem. Eng. Progress* **85**(10): 23-27 (1989). [2]
  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) [70]
  18. R. C. Willson, A. Z. Panagiotopoulos, and R. C. Reid, “High-pressure phase equilibria in ternary systems of propionic acid and water with CH<sub>4</sub>, SF<sub>6</sub>, CClF<sub>3</sub>, CF<sub>3</sub>H, or C<sub>2</sub>F<sub>6</sub>,” *J. Chem. Eng. Data* **36**: 290-293 (1991). DOI: [10.1021/jc00003a010](https://doi.org/10.1021/jc00003a010) [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) [92]
  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 Equil.* **66**: 41-55 (1991). DOI: [10.1016/.5046-W](https://doi.org/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 Equil.* **66**: 57-75 (1991). DOI: [10.1016/0378-3812\(91\)85047-X](https://doi.org/10.1016/0378-3812(91)85047-X) [38]
  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) [164]
  23. A. Z. Panagiotopoulos, “Molecular simulation of fluid-phase equilibria: simple, ionic and polymeric fluids,” *Fluid Phase Equil.* **76**: 97-112 (1992); erratum **92**: 313 (1994). DOI: [10.1016/0378-3812\(92\)85080-R](https://doi.org/10.1016/0378-3812(92)85080-R) [142]
  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](https://doi.org/10.1080/08...48258) [355]
  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) [57]
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  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) [12]

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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) [220]
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) [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 Equil.* **94**: 1-18 (1994). DOI: [10.1016/0378-3812\(94\)87049-7](https://doi.org/10.1016/0378-3812(94)87049-7) [25]
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) [116]
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) [18]
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) [225]
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) [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](https://doi.org/10.1209/0295-5075/27/7/010) [21]
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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 **129**: 311 (1997). DOI: [10.1016/0378-3812\(94\)02628-E](https://doi.org/10.1016/0378-3812(94)02628-E) [32]

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](https://doi.org/10.1002/aic.690411014) [21]
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) [72]
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) [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](https://doi.org/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](https://doi.org/10.1016/0378-3812(95)02894-3) [38]
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) [39]
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) [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](https://doi.org/10.1063/1.471406) [40]
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) [52]
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) [87]
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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) [130]
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) [194]
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) [71]
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) [250]
66. J.J. Potoff and A.Z. Panagiotopoulos, "Critical point and phase behavior of the pure fluid and a Lennard-Jones mixture," *J. Chem. Phys.* **109**: 10914-20 (1998). DOI: [10.1063/1.477787](https://doi.org/10.1063/1.477787) [372]
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