ATHANASSIOS Z. PANAGIOTOPOULOS

EDUCATION

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

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

Postdoctoral,
Physical Chemistry Laboratory, Oxford University, Oxford, UK (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)

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
Department Chair (2016-present), Susan Dod Brown Professor (2007-present), Professor (2000-2006), Director of Graduate Studies (2003-05, 2013-14)

SELECTED HONORS

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 AND ADVISORY BOARD MEMBERSHIPS

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

BOOK

Essential Thermodynamics, Drios Press, 2011 (undergraduate textbook)

REFEREED PUBLICATIONS

Bibliographic data as of Apr. 14, 2017: Google Scholar: 15,406 total citations, h=63; Web of Science: 12,263 total citations, h=56.

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," in K. C. Chao and R. L. Robinson (eds.), "Equations of State - Theories and Applications," *ACS Symposium Ser.*, **300**: 571-582 (1986). *[178]*

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 *[72]*

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 *[15]*

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 *[59]*

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/je00053a028 *[20]*

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). *[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 *[1,484]*

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 *[238]*

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 *[121]*

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 *[860]*

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 *[46]*

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 *[92]*

14. A. Z. Panagiotopoulos, "Gibbs-ensemble Monte Carlo simulations of phase equilibria in supercritical fluid systems," *ACS Symposium Ser.*, "Supercritical Fluid Science and Technology," K. P. Johnston and J. Penninger (eds.), **406**: 39-51 (1989). *[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). *[36]*
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 *[60]*
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).
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 *[77]*
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 *[30]*
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 *[138]*
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 *[107]*
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 *[281]*
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 *[53]*
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). *[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 *[54]*
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 *[6]*

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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 *[53]*
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33. A. Z. Panagiotopoulos, "Molecular simulation of phase equilibria," in *Supercritical Fluids - Fundamentals for Application*, E. Kiran. and J. M. H. Levelt Sengers (eds.), NATO ASI Series E, **273**, Kluwer Academic Publishers: Dordrecht, The Netherlands, pp. 411-437 (1994). *[18]*
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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 *[97]*
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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 *[188]*
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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). *[19]*
40. A. Z. Panagiotopoulos, "Monte Carlo simulation of phase coexistence for polymeric and ionic fluids," *Fluid Phase Equil.*, **104**, 185-194 (1995). DOI: 10.1016/0378-3812... *[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). *[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 *[106]*
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Dioxide from Molecular Simulation," *Fluid Phase Equil.*, **170**, 203-34 (2000). DOI: 10.1016/S0378-3812(00)00315-0 *[108]*

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RECENT INVITED SEMINARS AND LECTURES

"Simulations of Thermodynamic and Transport Properties for Aqueous Mixtures," QAFCO Conference, Doha, Qatar, March 3, 2015.

"Self-assembly in nanoparticle and polymer systems," Department of Chemical and Biomolecular Engineering, U. of Houston, March 30, 2015.

"Liquid-Liquid Transition in the ST2 Model for Water," Princeton Center for Theoretical Science "Ice Nucleation" workshop, Princeton U., April 23, 2015.

"Interactions, Phase Equilibria and Self-Assembly in Ionic Systems," Computational and Theoretical Chemistry Meeting, Annapolis, MD, April 27, 2015.

"Self-assembly in nanoparticle and polymer systems," Research Symposium in Honor of Prof. Claude Cohen, Cornell University, May 21, 2015.

"Simulations of aqueous electrolyte activity coefficients and solubilities," Workshop on Water under Extreme Conditions, Rome, Italy, June 10-12, 2015.

"Entropic Control over Nanoscale Colloidal Crystals," invited talk at the Plenary Session, Computational Molecular Science and Engineering Forum, AIChE Annual Meeting, Salt Lake City, UT, Nov. 8-13, 2015.

"Entropic Control over Nanoscale Colloidal Crystals," invited talk at the Symposium on Modeling and Theory-Driven Design of Soft Materials, MRS Fall Meeting, Boston, MA Nov. 29- Dec. 4, 2015.

"Molecular Simulation of Phase Equilibria: Progress and Challenges," Keith E. Gubbins Lecture, North Carolina State U., Jan. 11, 2016.

"Self-assembly in nanoparticle and polymer systems," Keith E. Gubbins Lecture, North Carolina State U., Jan. 12, 2016.

"Self-assembly in nanoparticle and polymer systems," Eduard Zintl Institute Colloquium, Technische Universität Darmstadt, Jan. 27, 2016.

"Simulations of Thermodynamic Properties and Self-Assembly in Aqueous Solutions," Institute of Physics, Johannes-Gutenberg Universität Mainz, Jan. 28, 2016.

"Simulations of mean ionic activity coefficients and solubilities in aqueous electrolyte solutions," Invited talk, Journal of Chemical Physics Editor's Choice session, APS March Meeting, Baltimore, Maryland, March 14–18, 2016.

"Bottom-up with a twist: A new approach for colloidal crystal assembly," Keynote Lecture, 90th ACS Colloid & Surface Science Symposium, Cambridge, MA, June 5-8, 2016.

"Simulations of Activity Coefficients and Solubilities for Aqueous Electrolytes: Why Are Our Models Off?" Invited talk at the "New Frontiers of Molecular Thermodynamics" session, AIChE Annual Meeting, San Francisco, CA, Nov. 12-18, 2016.

RECENT CONFERENCE PRESENTATIONS AND PAPERS

"Thermodynamic and Transport Properties for the H2O+CO2+NaCl System from Polarizable Force Fields," H. Jiang, O. A. Moultos, I. G. Economou, and A. Z. Panagiotopoulos, poster presentation at the PPEPPD International Conference, Porto, Portugal, May 22-26, 2016.

"Modeling of CO2 Solubility in Electrolyte Solutions and Brines Using Statistical Associating Fluid Theory," H. Jiang, I. G. Economoub and A. Z. Panagiotopoulos poster presentation at the PPEPPD International Conference, Porto, Portugal, May 22-26, 2016.

"Equilibrium crystal phases of triblock Janus particles," W. F. Reinhart and A. Z. Panagiotopoulos, poster presentation at the 90th ACS Colloid & Surface Science Symposium, Cambridge, MA, June 5-8, 2016.

"Axial dispersion of Brownian colloids in microfluidic channels," M. P. Howard, A. Gautam, A. Z. Panagiotopoulos, and A. Nikoubashman, poster presentation at the 90th ACS Colloid & Surface Science Symposium, Cambridge, MA, June 5-8, 2016.

"Self-Assembly of Directionally Interacting Spheres and Rods" N. A. Mahynski, W. Liu, O. Gang, A. Z. Panagiotopoulos, S. K. Kumar, AIChE Annual Meeting, San Francisco, CA, Nov. 12-18, 2016.

"Entropic Control over Nanoscale Colloidal Crystals", N. A. Mahynski, S. K. Kumar, At. Z. Panagiotopoulos AIChE

"Polymer-mediated Polymorphic Control over Open Colloidal Crystals" N. A. Mahynski, L. Rovigatti, C. N. Likos, A. Z. Panagiotopoulos, AIChE Annual Meeting, San Francisco, CA, Nov. 12-18, 2016.

"Modeling of CO2 Solubility in Electrolyte Solutions and Brines Using Statistical Associating Fluid Theory," H. Jiang, A. Z. Panagiotopoulos and I. G. Economou, AIChE Annual Meeting, San Francisco, CA, Nov. 12-18, 2016.

"A Gaussian-Charge Polarizable Model for Water," H. Jiang, O. A. Moultos, I. G. Economou, and A. Z. Panagiotopoulos, AIChE Annual Meeting, San Francisco, CA, Nov. 12-18, 2016.

"Calculation of Thermodynamic and Transport Properties of H2O+CO2+NaCl System," H. Jiang, O. A. Moultos, I. G. Economou, and A. Z. Panagiotopoulos, AIChE Annual Meeting, San Francisco, CA, Nov. 12-18, 2016.

"Open Crystals from Triblock Janus Colloids," W. F. Reinhart and A. Z. Panagiotopoulos, AIChE Annual Meeting, San Francisco, CA, Nov. 12-18, 2016.

"Efficient Neighbor List Calculation for Molecular Simulation of Colloidal Systems Using Graphics Processing Units," M. P. Howard, J. A. Anderson, A. Nikoubashman, S. C. Glotzer, and A. Z. Panagiotopoulos, AIChE Annual Meeting, San Francisco, CA, Nov. 12-18, 2016.

"Axial Dispersion of Brownian Colloids in Microfluidic Channels," M. P. Howard, A. Gautam, A. Z. Panagiotopoulos, and A. Nikoubashman, AIChE Annual Meeting, San Francisco, CA, Nov. 12-18, 2016.