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 Dec. 8, 2017: Google Scholar: 16,450 total citations, h=64; Web of Science: 12,938 total citations, h=58.

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). *[181]*
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 *[74]*
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 *[60]*
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 *[1,516]*
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 *[246]*
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 *[879]*
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 *[48]*
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). *[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 *[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 *[141]*
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 *[111]*
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 *[286]*
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]*
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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 *[11]*
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Dioxide from Molecular Simulation," *Fluid Phase Equil.*, **170**, 203-34 (2000). DOI: 10.1016/S0378-3812(00)00315-0 *[112]*

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RECENT INVITED SEMINARS AND LECTURES

"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.

"Molecular Dynamics and Monte Carlo Simulations," invited plenary at the ExxonMobil Longer-Range Research Meeting, Princeton, NJ, May 9, 2017.

"Simulations of Solubilities and Activity Coefficients in Aqueous Electrolyte Solutions," invoted talk at the DOE Computational and Theoretical Chemistry Meeting, Gaithersburg, MD, May 15-18, 2017.

"Electrolyte solutions: Simulation challenges and the quest for better models," keynote talk at the 29th European Symposium on Applied Thermodynamics, Bucharest, Romania, May 18-21, 2017.

"Polarizable models for water and aqueous solutions," invited talk at the Roma Tre Congress on Water Under Extreme Conditions, Rome, Italy, June 14-16, 2017.

"Simulations of homogeneous and structured polymeric nanoparticle formation through rapid solvent exchange," invited talk at the ACS 254th National Meeting, Washington, DC, Aug. 20, 2017.

"Evaporation-induced stratification and crystallization in drying colloidal / polymer systems," invited talk at the Joint EMGL/JMLG Meeting, Vienna, Austria, Sept. 11 – 14, 2017.

"Free Energies, Solubilities, and Nucleation Rates of Aqueous Electrolyte Solutions," Chemistry Colloquium, Brandeis University, Sept. 18, 2017.

"Free Energies, Solubilities, and Nucleation Rates of Aqueous Electrolyte Solutions," Chemical Engineering Colloquium, Univ. of California at Santa Barbara, Oct. 17, 2017.

RECENT CONFERENCE PRESENTATIONS AND PAPERS

"Anisotropic growth kinetics of triblock Janus colloids," W. F. Reinhart and A. Z. Panagiotopoulos, Gordon Research Conference on Crystal Growth & Assembly, U. of New England, Biddeford, ME, June 25 – 30, 2017.

"Understanding Evaporation-Induced Colloidal Crystallization by Machine Learning," W. F. Reinhart, M. P. Howard, A. Nikoubashman and A. Z. Panagiotopoulos, 91st ACS Colloid & Surface Science Symposium, New York, NY, July 9-1, 2017.

"Stratification dynamics in drying colloidal mixtures," M. P. Howard, A. Nikoubashman, and A. Z. Panagiotopoulos, 91st ACS Colloid & Surface Science Symposium, New York, NY, July 9-1, 2017.

"Open and Compact Self-Assembled Structures in Systems with Competing Interactions," A. P. Santos, J. Pękalski, A. Z. Panagiotopoulos, 91st ACS Colloid & Surface Science Symposium, New York, NY, July 9-1, 2017.

"Fabrication of homogeneous and structured polymeric nanoparticles through rapid solvent exchange," A. Nikoubashman, N. Li, V.E. Lee, C. Sosa, R.K. Prud'homme, R.D. Priestley, and A.Z. Panagiotopoulos, Liquid Matter Conference, Ljubljana, Slovenia, July 17-21, 2017.

"Evaporation-induced nucleation and growth of colloidal crystals," W. F. Reinhart, M. P. Howard, and A. Z. Panagiotopoulos, Thermodynamics 2017, Edinburgh, U.K., Sept. 5-8, 2017.

"Structured Nanoparticles from the Self-Assembly of Polymer Blends through Rapid Sol-vent Exchange," N. Li, A. Z. Panagiotopoulos and A. Nikoubashman, paper 445f, AIChE Meeting, Minneapolis, MN, Oct. 29 – Nov. 3, 2017.

"Anisotropic Growth Kinetics of Triblock Janus Colloids," W. F. Reinhart and A. Z. Panag-iotopoulos, paper 683g, AIChE Meeting, Minneapolis, MN, Oct. 29 – Nov. 3, 2017.

"Evaporation-Induced Assembly of Colloidal Crystals," M. P. Howard, W. F. Reinhart, A. Nikoubashman and A. Z. Panagiotopoulos, paper 704c, AIChE Meeting, Minneapolis, MN, Oct. 29 – Nov. 3, 2017.

"Concentration Effects in Simulations of Non-Ionic and Ionic Surfactant Micellization," A. P. Santos and A. Z. Panagiotopoulos, paper 704g, AIChE Meeting, Minneapolis, MN, Oct. 29 – Nov. 3, 2017.

"Massively-Parallel Mesoscale Hydrodynamics on Graphics Processing Units," M. P. Howard, A. Nikoubashman and A. Z. Panagiotopoulos, paper 736g, AIChE Meeting, Minneapolis, MN, Oct. 29 – Nov. 3, 2017

"Machine Learning for Autonomous Crystal Structure Identification," W. F. Reinhart, A. W. Long, M. P. Howard, A. L. Ferguson, and A. Z. Panagiotopoulos, paper 747a, AIChE Meeting, Minneapolis, MN, Oct. 29 – Nov. 3, 2017.

"Stratification dynamics in drying colloidal mixtures," M. P. Howard, A. Nikoubashman, and A. Z. Panagiotopoulos, paper 749g, AIChE Meeting, Minneapolis, MN, Oct. 29 – Nov. 3, 2017.

"Evaporation-induced colloidal assembly," M. P. Howard, W. F. Reinhart, A. Nikoubashman, A. Z. Panagiotopoulos, PICSciE Research Computing Day, Princeton, NJ, Nov. 7, 2017.