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Education

Ph.D., December 1988, Department of Chemical Engineering, University of Pennsylvania, Philadelphia PA. Thesis: *Theoretical and Computer Simulation Studies of Mixtures of Very Many Components*. Advisor: Professor Eduardo D. Glandt

B.S., May 1983 (with University Honors), Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA

Professional Experience

Walter E. Schmid Professor, 2021-present, SUNY Distinguished Professor, 2012-present; Department Chair, 2006-2012; UB Distinguished Professor, 2004-2012; Professor, 1998-2004; Associate Professor, 1994-1998; Assistant Professor, 1989-1994; Department of Chemical Engineering (Department of Chemical and Biological Engineering as of November 2003); University at Buffalo, The State University of New York
Department co-Chair, July 2010 - June 2012, Department of Biomedical Engineering, University at Buffalo, The State University of New York

Visiting Research Professor, July 1996 - June 1997; Department of Chemical Engineering; University of Tennessee
Sponsor: Professor Peter Cummings

Visiting Researcher, May-June 1992; FOM Institute for Atomic and Molecular Physics; Amsterdam, The Netherlands
Sponsor: Dr. Daan Frenkel

Postdoctoral Fellow, 1988-89; Department of Chemical and Biochemical Engineering; Rutgers, The State University of New Jersey; Piscataway, NJ
Research Topic: *Molecular Dynamics Studies of Antigen-Antibody Interactions*
Advisor: Professor Martin Yarmush

Research Interests

Molecular and engineering thermodynamics. Calculation of free energy and phase equilibria by molecular simulation. Applications to phase behavior in solids and analysis of crystal stability. Calculation of cluster integrals, with application to modeling of dense gases and supercritical fluids. Integration of cluster-based methods with *ab initio* computational chemistry. Development and application of object-oriented software for molecular modeling.

Honors and Awards

Distinguished Postdoc Mentor Award, 2019
Fellow of the American Association for the Advancement of Science, 2014
Fellow of the American Institute of Chemical Engineers, 2014
SUNY Distinguished Professor, 2012
David Himmelblau Award for Innovations in Computer-Based Chemical Engineering Education, CAST Division of AIChE, 2012
Profiled in *Chemical Engineering Education*, Summer 2012
Schlumberger Lecturer, University of Alberta, 2009
Johansen-Crosby Lecturer in Chemical Engineering, Michigan State University, 2008
AIChE Area1a Keynote Lecturer, 2007
Carnegie Mellon University Alumni Achievement Award, 2007
Jacob F. Schoellkopf Medal, Western New York Section of the ACS, 2007
SUNY Chancellor's Award for Excellence in Research and Creative Activity, 2004
John M. Prausnitz Award in Applied Chemical Thermodynamics, 2004
UB Exceptional Scholar Award (Sustained Achievement), 2002
SUNY Chancellor's Award for Excellence in Teaching, 1994
Dow Outstanding New Faculty Award of the ASEE, 1994
Presidential Young Investigator Award, 1990-95
General Electric Forgivable Loan, 1987-88
Research Fellowship, AMOCO Foundation, 1986-87
DuPont Ph.D. Fellowship in Chemical Engineering, 1983-87
Tau Beta Pi, 1982

Refereed Publications

ResearcherID: E-8102-2011; ORCID iD: 0000-0002-2530-8816

1. D.A. Kofke, "Origins of the Failure of the Activity Virial Series", *J. Phys. Chem. B*, **127**, 3690-3700 (2023). DOI: 10.1021/acs.jpcb.3c00807
2. A. Bansal, A.J. Schultz, J. Douglas, and D.A. Kofke, "Probabilistic Computations of Virial Coefficients of Polymeric Structures Described by Rigid Configurations of Spherical Particles: A Fundamental Extension of the ZENO Program", *J. Chem. Phys.* **157**, 224801 (2022). DOI: 10.1063/5.0127465.
3. A.J. Schultz and D.A. Kofke, "Virial equation of state as a New Frontier for Computational Chemistry" (Invited Perspective article), *J. Chem. Phys.*, **157**, 190901 (2022). DOI: 10.1063/5.0113730. Selected as a *2022 Editors' Choice*.
4. S.G. Moustafa, A.J. Schultz, and D.A. Kofke, "Reformulation of Expressions for Thermoelastic Properties of Crystals using Harmonic Mapping", *Phys. Rev. B*, **106**, 104105 (2022). DOI: 10.1103/PhysRevB.106.104105.
5. N. Gokul, A.J. Schultz, D.A. Kofke, "Speed of Sound in Helium-4 from Ab Initio Acoustic Virial Coefficients" *J. Chem. Eng. Data* **66**, 3258-3281 (2021). DOI: 10.1021/acs.jced.1c00328
6. A. Bansal, A.J. Schultz, and D.A. Kofke, "Evaluation of Osmotic Virial Coefficients via Restricted Gibbs Ensemble Simulations, with Support from Gas-Phase Mixture Coefficients", *J. Phys. Chem. B*, **125**, 7262-7272 (2021). DOI: 10.1021/acs.jpcb.1c02100

7. S.G. Moustafa, A. Purohit, A.J. Schultz, and D.A. Kofke, "pyHMA: A VASP post-processor for precise measurement of crystalline anharmonic properties using harmonically mapped averaging", *Comput. Phys. Commun.* **258**, 107554 (2021). DOI: 10.1016/j.cpc.2020.107554
8. A.J. Schultz and D.A. Kofke, "Identifying and estimating bias in overlap-sampling free-energy calculations", *Mol. Sim.* **47**(5), 379-389 (2021). DOI: 10.1080/08927022.2020.1758695
9. N. Gokul, A.J. Schultz, and D.A. Kofke, "Properties of Supercritical N2, O2, CO2, and NH3 Mixtures from the Virial Equation of State", *AIChE J.* **67**(3), e17072 (2020). DOI: 10.1002/aic.17072
10. Apoorva Purohit, Andrew J. Schultz, and David A. Kofke, "Implementation of harmonically mapped averaging in LAMMPS, and effect of potential truncation on anharmonic properties", *J. Chem. Phys.* **152**, 014107 (2020), Selected by journal as "Editor's Pick". DOI: 10.1063/1.5129942
11. Richard J Wheatley, Andrew J Schultz, Hainam Do, Navneeth Gokul, and David A Kofke, "Cluster integrals and virial coefficients for realistic molecular models", *Phys. Rev. E* **101**, 051301(R) (2020). DOI: 10.1103/PhysRevE.101.051301
12. J. Richard Elliott, Andrew J. Schultz, and David A. Kofke, "Combined Temperature and Density Series for Fluid-Phase Properties. 2. Lennard-Jones Spheres", *J. Chem. Phys.* **51**(20), 204501 (2019). DOI: 10.1063/1.5126281
13. Andrij Trokhymchuk, Andrew J. Schultz, and David A. Kofke, "Alternative ensemble averages in molecular dynamics simulation of hard spheres", *Molec. Phys.* **117**(23-24), 3734-3753 (2019). DOI: 10.1080/00268976.2019.1664779
14. R.A. Messerly, N. Gokul, A.J. Schultz, D.A. Kofke, and A.H. Harvey, "Molecular calculation of the critical parameters of classical helium", *J. Chem. Eng. Data*, **65**(3), 1028-1037 (2019). DOI: 10.1021/acs.jced.9b00443
15. A.J. Schultz and D.A. Kofke, "Virial coefficients of helium-4 from ab initio-based molecular models", *J. Chem. Eng. Data* **64**(9) 3742-3754 (2019). DOI 10.1021/acs.jced.9b00183
16. A.J. Schultz and D.A. Kofke, "Alternatives to conventional ensemble averages for thermodynamic properties," *Curr. Opin. Chem. Eng.* **23**, 70-76 (2019). DOI: 10.1016/j.coche.2019.02.002
17. A. Purohit, A.J. Schultz, and D.A. Kofke, "Force-sampling methods for density distributions as instances of mapped averaging", *Molec. Phys.* **117**(20), 2822-2829 (2019). DOI: 10.1080/00268976.2019.1572243

18. A. Bansal, A.J. Schultz, and D.A. Kofke, J. Hachmann, "Machine Learning from Heteroscedastic Data: Second Virial Coefficients of Alkane Isomers", *J. Phys. Chem. B* (submitted) (2023).

19. A.J. Schultz and D.A. Kofke, "Comprehensive high-precision high-accuracy equation of state and coexistence properties for classical Lennard-Jones crystals and low-temperature fluid phases", *J. Chem. Phys.* **149**, 204508 (2018). Selected as a *2018 Editor's Choice* article, one of 72 most innovative and influential articles of 2018. DOI: 10.1063/1.5053714
20. S.G. Moustafa, A.J. Schultz, and D.A. Kofke, "Effects of thermostatting in molecular dynamics on anharmonic properties of crystals: Application to fcc Al at high pressure and temperature", *J. Chem. Phys.* **149**, 124109 (2018). Selected by journal as "Editor's Choice". DOI: 10.1063/1.5043614

21. A.J. Schultz, S.G. Moustafa, and D.A. Kofke, "No system-size anomalies in entropy of bcc iron at Earth's inner-core conditions", *Sci. Rep*. **8**, 7295 (2018). DOI: 10.1038/s41598-018-25419-3
22. A. Purohit, A.J. Schultz, S.G. Moustafa, J.R. Errington, and D.A. Kofke, "Free energy and concentration of crystalline vacancies by molecular simulation", *Mol. Phys.* **116**(21-22) 3027-3041 (2018). DOI: 10.1080/00268976.2018.1481542
23. W. Lin, A.J. Schultz, and D.A. Kofke, "Electric-field mapped averaging for the dielectric constant", *Fluid Phase Equil.* **470**, 17-24 (2018). DOI: 10.1016/j.fluid.2018.01.036.
24. M.E. Irrgang, M. Engel, A.J. Schultz, D.A. Kofke, and S.C. Glotzer, "Virial coefficients and equations of state for hard-polyhedron fluids", *Langmuir*, **33**(42), 11788-11796 (2017).
25. S.G. Moustafa, A.J. Schultz, E. Zurek, and D.A. Kofke, "Accurate and precise *ab initio* anharmonic free-energy calculations for metallic crystals. Application to hcp Fe at high temperature and pressure," *Phys. Rev. B* **96**, 014117 (2017). DOI: 10.1103/PhysRevB.96.014117
26. S. Yang, A.J. Schultz, and D.A. Kofke, "Evaluation of second and third dielectric virial coefficients for non-polarizable molecular models", *Molec. Phys*. **115**(8), 991-1003 (2017). DOI 10.1080/00268976.2017.1301585
27. R. Subramanian, A.J. Schultz, and D.A. Kofke, "Quantum virial coefficients of molecular nitrogen," *Molec. Phys.* **115**(7) 869-878 (2017). DOI 10.1080/00268976.2017.1290842
28. R. Subramanian, A.J. Schultz, and D.A. Kofke, "Direct orientation sampling of diatomic molecules for path integral Monte Carlo calculation of fully quantum virial coefficients," *J. Chem. Phys.* **146**, 094105 (2017). DOI 10.1063/1.4977597
29. S.G. Moustafa, A.J. Schultz, and D.A. Kofke, "Harmonically assisted methods for computing the free energy of classical crystals by molecular simulation: A comparative study," *J. Chem. Theory Comput.* **13**(2), 825-834 (2016). DOI: 10.1021/acs.jctc.6b01082
30. S. Yang, A.J. Schultz, and D.A. Kofke, "Thermodynamic properties of supercritical CO_2/CH_4 mixtures from the virial equation of state", *J. Chem. Eng. Data* **61**(12), 4296-4212 (2016). DOI 10.1021/acs.jced.6b00702
31. H. Do, C. Feng, A.J. Schultz, D.A. Kofke, and R.J. Wheatley, "Calculation of high-order virial coefficients for the square-well potential", *Phys. Rev. E.* **94**(1), 013301 (2016) DOI 10.1103/PhysRevE.94.013301
32. A.J. Schultz, S.G. Moustafa, W. Lin, S.J. Weinstein, and D.A. Kofke, "Reformulation of ensemble averages via coordinate mapping", *J. Chem. Theory Comput.*, **12**, 1491-1498 (2016) DOI 10.1021/acs.jctc.6b00018
33. A.J. Schultz and D.A. Kofke, "Vapor-phase metastability and condensation via the virial equation of state with extrapolated coefficients", *Fluid Phase Equil*. **409**, 12-18 (2016).
34. S.G. Moustafa, A.J. Schultz, and D.A. Kofke, "Very fast averaging of thermal properties of crystals by molecular simulation", *Phys. Rev. E* **92**(4), 043303 (2015).
35. J.R. Elliott, A.J. Schultz, and D.A. Kofke, "Combined temperature and density series for fluid-phase properties: 1. Square-well spheres", *J. Chem. Phys.* **143**, 114110 (2015).
36. N.S. Barlow, A.J. Schultz, S.J. Weinstein, and D.A. Kofke, "Communication: Analytic continuation of the virial series through the critical point using parametric approximants", *J. Chem. Phys.* **143**, 071103 (2015).
37. A.J. Schultz, D.A. Kofke, and A.H. Harvey, "Molecular-Based Virial Coefficients of CO_2-H_2O Mixtures", *AIChE J*. **61**(9), 3029-3037 (2015).
38. C. Feng, A.J. Schultz, V. Chaudhary, and D.A. Kofke, "Eighth to Sixteenth Virial Coefficients of the Lennard-Jones Model", *J. Chem. Phys*. **143**, 044504 (2015).
39. J.H. Yang, A.J. Schultz, J.R. Errington, and D.A. Kofke, "The rate of convergence of the virial series in confined systems", *Mol. Phys.* **113**(9-10), 1179-1189 (2015).

40. S.G. Moustafa, A.J. Schultz, and D.A Kofke, "Effects of finite size and proton disorder on lattice-dynamics estimates of the free energy of clathrate hydrates", *I&EC Research* **54**, 4487-4496 (2015).
41. A.J. Schultz and D.A. Kofke, "Etomica: An object-oriented framework for molecular simulation", *J. Comp. Chem.* **36**(8), 573-583 (2015). (doi 10.1002/jcc.23823)
42. A.J. Schultz and D.A. Kofke, "Quantifying computational effort required for stochastic averages", *J. Chem. Theory Comput.* **10**(12), 5229-5234 (2014).
43. S. Yang, A.J. Schultz, D.A. Kofke, and A.H. Harvey, "Interpreting gas-saturation vapor pressure measurements using virial coefficients derived from molecular models", *J. Chem. Eng. Data* **59**(10), 3183-3192 (2014).
44. N. Barlow, A.J. Schultz, D.A. Kofke, and S.J. Weinstein, "Critical isotherms from virial series using asymptotically consistent approximants", *AIChE J.* **60**(9), 3336-3349 (2014).
45. A.J. Schultz and D.A. Kofke, "Fifth to eleventh virial coefficients of hard spheres", *Phys. Rev. E* **90**, 023301 (2014).
46. S.G. Moustafa, A.J. Schultz, and D.A. Kofke, "A Comparative study of methods to compute the free energy of an ordered assembly by molecular simulation", *J. Chem. Phys.* **139**, 084105 (2013).
47. H.M. Kim, A.J. Schultz, and D.A. Kofke, "Second through fifth virial coefficients for model methane-ethane mixtures", *Fluid Phase Equil.* **351**, 69-73 (2013).
48. J.H. Yang, A.J. Schultz, J.R. Errington, and D.A. Kofke, "Calculation of inhomogeneous-fluid cluster expansions with application to the hard-sphere/hard-wall system", *J. Chem. Phys.* **138**, 134706 (2013).
49. N. Barlow, A.J. Schultz, V. Chaudhary, and D.A. Kofke, "Mayer sampling Monte Carlo calculation of virial coefficients on graphics processors", *Molec. Phys*. **111**(4), 535-543 (2013).
50. H.M. Kim, A.J. Schultz, and D.A. Kofke, "A virial equation of state of water based on Wertheim's association theory", *J. Phys. Chem. B* **116**, 14078-14088 (2012).
51. N. Barlow, A.J. Schultz, S.J. Weinstein, and D.A. Kofke, "An asymptotically consistent approximant method with application to soft- and hard-sphere fluids", *J. Chem. Phys.* **137**, 204102/1-13 (2012).
52. K.R.S. Shaul, A.J. Schultz, and D.A. Kofke, "Path-integral Mayer-sampling calculations of the quantum Boltzmann contribution to virial coefficients of helium-4", *J. Chem. Phys.* **137**, 184101/1-12 (2012).
53. K.R.S. Shaul, A.J. Schultz, D.A. Kofke, and M.R. Moldover, "Semiclassical fifth virial coefficients for improved *ab initio* helium-4 standards", *Chem. Phys. Lett.* **531**, 11-17 (2012). (judged by the journal to be within top 5% of submissions, and so designated as "Editor's Choice").
54. K.R.S. Shaul, A.J. Schultz, A. Perera, and D.A. Kofke, "Integral equation theories and Mayer-sampling Monte Carlo: A tandem approach for computing virial coefficients of simple fluids", *Molec. Phys.* **109**(20) 2395-2406 (2011).
55. A.J. Schultz and D.A. Kofke, "Algorithm for constant pressure Monte Carlo simulation of crystalline solids", *Phys. Rev. E* **84**, 046712/1-6 (2011).
56. K.R.S. Shaul, A.J. Schultz, and D.A. Kofke, "Mayer sampling Monte Carlo calculations of uniquely flexible contributions to virial coefficients", *J. Chem. Phys.* **135**, 124101/1-9 (2011).
57. T.B. Tan, A.J. Schultz, and D.A. Kofke, "Efficient calculation of α- and β-nitrogen free energies and coexistence conditions via overlap sampling with targeted perturbation", *J. Chem. Phys*. **135**, 044125/1-13 (2011).

58. M.S. Sellers, A.J. Schultz, C. Basaran, and D.A. Kofke, "Effect of Cu and Ag solute segregation on β-Sn grain boundary diffusivity", *J. Appl. Phys.* **110**, 013528/1-9 (2011).
59. M.S. Sellers, A.J. Schultz, D.A. Kofke, and C. Basaran, "Solute effects on β-Sn grain boundary energy and shear stress", *J. Nanomechanics and Micromechanics* **1**(1), 41 (2011).
60. T.B. Tan, A.J. Schultz, and D.A. Kofke, "Virial coefficients, equation of state, and solid-fluid coexistence for the soft-sphere model", *Molec. Phys.* **109**(1), 123-132 (2011).
61. K.R.S. Shaul, A.J. Schultz, and D.A. Kofke, "Mayer-sampling Monte Carlo calculations of methanol virial coefficients", *Molec. Sim*. **36**(15), 1282-1288 (2010).
62. A.J. Schultz, K.R.S. Shaul, S. Yang, and D.A. Kofke, "Modeling solubility in supercritical fluids via the virial equation of state", *J. Supercrit. Fluids* **55**(2), 479-484 (2010).
63. T.B. Tan, A.J. Schultz, and D.A. Kofke, "Efficient calculation of temperature dependence of solid-phase free energies by overlap sampling coupled with harmonically targeted perturbation", *J. Chem. Phys.* **133**(13), 134104/1-11 (2010).
64. A.J. Schultz and D.A. Kofke, "Virial coefficients of model alkanes", *J. Chem. Phys.* **133**(10), 104101/1-7 (2010). (Highlighted on cover of issue).
65. H.M. Kim, A.J. Schultz, and D.A. Kofke, "Molecular-based modeling of associating fluids via calculation of Wertheim cluster integrals", *J. Phys. Chem. B* **114**, 11515-11524 (2010).
66. T.B. Tan, A.J. Schultz, and D.A. Kofke, "Suitability of umbrella- and overlap-sampling methods for calculation of solid-phase free energies by molecular simulation", *J. Chem. Phys.* **132**, 214103/1-11 (2010).
67. M. Sellers, A.J. Schultz, C. Basaran, and D.A. Kofke, "β-Sn grain boundary structure and self-diffusivity via molecular dynamics simulations", *Phys. Rev. B* **81**, 134111/1-10 (2010).
68. K.R.S. Shaul, A. J. Schultz, and D.A. Kofke, "Effect of truncation and shift on virial coefficients of Lennard-Jones potentials", *Collect. Czech. Chem. Commun.* **75**, 447-462 (2010) [doi: 10.1135/cccc2009113].
69. A.J. Schultz, R. Henda, and D.A. Kofke, "Interactive module for the molecular simulation of the mechanical response of a self-assembled monolayer at a golden interface", *2009 Bulletin of the Australian Institute of High Energetic Materials*, V. Stamatov, Ed. (USBN: 978-0-9806811-3-0), **1**, 46-56 (2010).
70. M.S. Sellers, A.J. Schultz, C. Basaran, and D.A. Kofke, "Atomistic modeling of β-Sn surface energies and adatom diffusivity", *App. Surf. Sci*, **256**, 4402-4407 (2010).
71. A.J. Schultz and D.A. Kofke, "Sixth, seventh and eighth virial coefficients of the Lennard-Jones model", *Mol. Phys.*, **107**(21), 2309-2318 (2009).
72. S. Li, M.S. Sellers, C. Basaran, A.J. Schultz, and D.A. Kofke, "Lattice strain due to an atomic vacancy", *Int. J. of Molecular Sciences* **10**(6), 2798-2808 (2009).
73. A.J. Schultz and D.A. Kofke, "Virial coefficients of Lennard-Jones mixtures", *J. Chem. Phys.* **130**, 224104/1-9 (2009).
74. A.J. Schultz and D.A. Kofke, "Interpolation of virial coefficients", *Molec. Phys.* **107**(14), 1431-1436 (2009).
75. K.M. Benjamin, A.J. Schultz, and D.A. Kofke, "Fourth and fifth virial coefficients of polarizable water", *J Phys. Chem. B* **113**(22), 7810-7815 (2009); Erratum: **114**(12), 4388 (2010).
76. J.R. Errington and D.A. Kofke, "Calculation of surface tension through area sampling", *J. Chem. Phys*. **127**, 174709/1-12 (2007).
77. K.E. Benjamin, A.J. Schultz, and D.A. Kofke, "Virial coefficients of polarizable water: Applications to thermodynamic properties and molecular clustering", *J. Phys. Chem. C* **111**(43), 16021-16027 (2007).

78. K.E. Benjamin, J.K. Singh, A.J. Schultz, and D.A. Kofke, "Higher-order virial coefficients of water models", *J. Phys. Chem. B* **111**(39), 11463-11473 (2007).
79. D.A. Kofke, "On the sampling requirements for exponential-work free-energy calculations", *Mol. Phys.* **104**(22-24), 3701-3708 (2006).
80. K. M. Benjamin, A. J. Schultz, and D.A. Kofke, "Gas-Phase molecular clustering of TIP4P and SPC/E water models from higher-order virial coefficients", *Ind. Eng. Chem. Res.* **45**(16) 5566-5573 (2006).
81. S. Wierzchowski, Z.H. Fang, D.A. Kofke, and J.L. Tilson, "Three-body effects in hydrogen fluoride: Survey of potential energy surfaces", *Mol. Phys.* **104**(4), 503-513 (2006).
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83. D. Wu and D.A. Kofke, "Phase-space overlap measures. 1. Fail-safe bias detection in free energies calculated by molecular simulation", *J. Chem. Phys.* **123**, 054103/1-10 (2005).
84. A. Kone and D.A. Kofke, "Selection of temperature intervals for parallel-tempering simulations", *J. Chem. Phys.* **122**, 206101/1-2 (2005).
85. D. Wu and D.A. Kofke, "Rosenbluth sampled nonequilibrium work method for calculation of free energies in molecular simulation", *J. Chem. Phys.* **122**, 204104/1-13 (2005).
86. S.K. Kwak and D.A. Kofke, "Effect of monovacancies on the relative stability of fcc and hcp hard-sphere crystals", *J. Chem. Phys.* **122**, 176101/1-2 (2005).
87. J.K. Singh and D.A. Kofke, "Molecular simulation study of the effect of pressure on the vapor-liquid interface of the square-well fluid", *Langmuir* **21**, 4218-4226 (2005).
88. S.K. Kwak and D.A. Kofke, "Evaluation of bridge-function diagrams via Mayer sampling Monte Carlo simulation", *J. Chem. Phys.* **122**, 104508/1-7 (2005).
89. S. Wierzchowski and D.A. Kofke, "Trimer based polarization as a multibody molecular model. Application to hydrogen fluoride", *J. Amer. Chem. Soc.*, **127**, 690-698 (2005).
90. D.A. Kofke, "Free energy methods in molecular simulation", *Fluid Phase Equil.* **228-229C**, 41-48 (2005).
91. S.K. Kwak and D.A. Kofke, "Elastic constants and effect of strain on monovacancy concentration in FCC hard-sphere crystals", *Phys. Rev. B* **70**, 214113 1-6 (2004).
92. D. Wu and D.A. Kofke, "Asymmetric bias in free-energy perturbation measurements using two Hamiltonian-based models", *Phys. Rev. E* **70**, 066702/1-11 (2004).
93. J.K. Singh and D.A. Kofke, "Molecular simulation study of the effect of molecular association on vapor-liquid interfacial properties", *J. Chem. Phys.* **121**(19) 9574-9580 (2004).
94. D. Wu and D.A. Kofke, "Model for small-sample bias of free-energy calculations applied to Gaussian-distributed nonequilibrium work measurements", *J. Chem. Phys.* **121**(18) 8742-8747 (2004).
95. D.A. Kofke, "Comment on 'The incomplete beta function law for parallel tempering sampling of classical canonical systems'", *J. Chem. Phys.* **121**(2) 1167 (2004).
96. J.K. Singh and D.A. Kofke, "Mayer sampling: Calculation of cluster integrals using free-energy perturbation methods" *Phys. Rev. Lett.* **92**(22) 220601 (2004). Erratum: **95**, 249903 (2005).
97. N. Lu, D. Wu, T.B. Woolf and D.A. Kofke, "Using overlap and funnel sampling to obtain accurate free energies from non-equilibrium work measurements", *Phys. Rev. E* **69** 057702 (2004); selected also to appear in *Virt. J. Biol. Phys. Res.* **7**(11) (2004).
98. J. Adhikari and D.A. Kofke, "Molecular simulation study of miscibility of ternary and quaternary InGaAlN alloys", *J. Appl. Phys.* **95**(11) 6129-6137 (2004).
99. D.A. Kofke, "Getting the most from molecular simulation", *Mol. Phys.* **102**(4) 405-420 (2004).

100. J. Adhikari and D.A. Kofke, "Molecular simulation study of miscibility in $In_xGa_{1-x}N$ ternary alloys", *J. Appl. Phys.* **95**(8) 4500-4502 (2004).
101. J.K. Singh and D.A. Kofke, "Molecular simulation study of the vapor-liquid interfacial behavior of a dimer-forming associating fluid", *Mol. Sim.* **30**(6) 343-351 (2004).
102. S. Wierzchowski and D.A. Kofke, "Liquid-phase activity coefficients for saturated HF/H_2O mixtures with vapor-phase nonidealities described by molecular simulation", *Ind. Eng. Chem. Res.*, **43**(1) 218-227 (2004).
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164. D.B. Kitchen, F. Hirata, J.D. Westbrook, R. Levy, D. Kofke, and M. Yarmush, "Conserving Energy During Molecular Dynamics Simulations of Water, Proteins, and Proteins in Water", *J. Comp. Chem.* **11**(10), 1169-1180 (1990).
165. D.A. Kofke and E.D. Glandt, "A Composition Density Functional Theory for Mixtures Based upon an Infinitely Polydisperse Reference. 2. Freezing in Hard Sphere Mixtures", *J. Chem. Phys.* **92**(7), 4417-4425 (1990).
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Edited Books

Foundations of Molecular Modeling and Simulation. Select Papers from FOMMS 2015, R.Q. Snurr, C.S. Adjiman, and D.A. Kofke (eds.). Springer, Singapore (2016).

Chapters in Books

1. D.A. Kofke and D. Frenkel, "Perspective: Free energies and phase equilibria", pp. 683-705 in *Handbook of Materials Modeling*, S. Yip, editor, (Springer, Dordrecht, 2005).
2. D.A. Kofke and J.A. Henning, "Thermodynamic integration along coexistence lines", pp. 99-127, Chapter 4 in Molecular Dynamics. From Classical to Quantum Methods, J. Seminario and P. Balbuena, eds., Volume 7 of Series in Theoretical and Computational Chemistry, Prof. P. Politzer, series editor. Elsevier Science Publishers, Amsterdam (1999).

Refereed Conference Proceedings

1. Ramachandran Subramanian, A.J. Schultz, and D.A. Kofke, "Quantum Virial Coefficients via Path Integral Monte Carlo with Semi-classical Beads", in *Foundations of Molecular Modeling and Simulation: Select Papers from FOMMS 2015*, Randall Q Snurr et al. (Eds), 93-106 (2016). DOI 10.1007/978-981-10-1128-3_6.

2. C. Feng, A.J. Schultz, V. Chaudhary, and D.A. Kofke, "Mixed-precision models for calculation of high-order virial coefficients on GPUs", 21st Annual International Conference on High Performance Computing (23% acceptance rate).
3. R. Henda, A.J. Schultz, and D.A. Kofke, "A Computer module for the simulation of the mechanical behaviour of self-assembled films on solid substrates", 2009 Interdisciplinary Conference on Chemical, Mechanical and Materials Engineering (2009 ICCMME), Published by The Australian Institute of High Energetic Materials (ABN 68 126 426 917), V. Stamatov, ed. (2010).
4. J.P. Walters, V. Balu, V. Chaudhary, D.A. Kofke, and A.J. Schultz, "Accelerating molecular dynamics simulations with GPUs", Proceedings of the 21st International Society for Computers and their Applications, Parallel and Distributed Computing and Communication System (ISCA-PDCCS'08), New Orleans, LA, 2008.
5. H. Bucher, A.J. Schultz, and D.A. Kofke, "An Eclipse-based environment for molecular simulation", Proceedings of the 2005 Object oriented programming systems languages and applications (OOPSLA) workshop on Eclipse technology eXchange, San Diego, CA, 130-134 (2005). (18% acceptance rate)
6. D.A. Kofke and E.D. Glandt, "Calculation of Phase Diagrams of Reactive Mixtures by Computer Simulation", Proceedings of the International Symposium on Thermodynamics in Chemical Engineering and Industry, Beijing, May 1988.

Other Publications

1. D.A. Kofke, J.I. Siepmann, R.D. Chirico, M. Kroon, P.M. Mathias, G. Sadowski, J. Wu, and J.F. Brennecke, "Editorial: Molecular modeling and simulation in JCED," *J. Chem. Eng. Data*, **61**(1), 1-2 (2016). DOI: 10.1021/acs.jced.5b01054.
2. D.A. Kofke, "Stirred Pots" note on anagrams of 'Thermodynamics', Chemical Engineering Education, Summer 1996, p. 183.
3. D.A. Kofke, "Chemical Engineering at the State University of New York at Buffalo", Chemical Engineering Education, Winter 1994.
4. Book review of: Dynamics and Thermodynamics in Hierarchically Organized Systems: Applications in Physics, Biology and Economics by Pierre Auger, *Math. Biosci.* **103**, 307 (1991).

Research Grants Awarded

Current

National Science Foundation (OAC-1739145), "SI2-SSE: Infrastructure Enabling Broad Adoption of New Methods That Yield Orders-of-Magnitude Speedup of Molecular Simulation Averaging", Amount: $499,734. Role: PI of 2 investigators. Term of award: 10/01/17 – 09/30/20.

Expired

U.S. Department of Commerce (NIST): "Software Module for the Calculation of Virial Coefficients of Non-rigid Macromolecules", Amount: $41,981. Role: PI. Term of award: 05/01/2022 – 04/30/2023.

U.S. Department of Commerce (NIST): “A Software Module for Calculation of Virial Coefficients of Macromolecules”, Amount: $33,545. Role: PI. Term of award: 09/01/2018 – 08/31/2019.

National Science Foundation (CBET-1510017), “UNS: Detailed molecular-thermodynamic methods for high-precision calculation of condensation, criticality, and supercritical behaviors of fluids and fluid mixtures”, Amount: $324,613. Role: PI of 2 investigators. Term of award: 06/15/15 – 05/31/21.

National Science Foundation (CHE-1464581), “CDS&E: Development and application of cluster-integral methods for dispersions and complex solutions”, Amount: $360,000. Role: PI of 2 investigators. Term of award: 06/15/15 – 05/31/18.

U.S. Department of Commerce (NIST): “Low-temperature virial coefficients and the critical point of classical helium”, Amount: $10,000. Role: PI. Term of award: 10/01/2017 – 09/30/2018.

National Science Foundation (CHE-1027963), “CDI Type II: New cyber-enabled strategies to realize the promise of quantum chemistry as a far-reaching tool for engineering applications”, Amount: $1,426,482. Role: PI of 4 investigators. Term of award: 10/01/10 – 09/30/16.

Petroleum Research Fund of the American Chemical Society, “A Comprehensive Molecular-Based Study of the Stability of Clathrate Hydrates”, Amount: $100,000. Role: PI. Term of award: 07/01/13 – 08/31/15.

University at Buffalo Innovative Micro-Programs Accelerating Collaboration in Themes (IMPACT), “Collaboration to Develop Key Capability Needed for Materials Innovation”, Amount: $33,254. Role: PI of 2 investigators. Term of award: 04/15/14 – 04/14/15.

National Science Foundation (DBI-0959870), “MRI-R2: Acquisition of a Data Intensive Supercomputer for Innovative and Transformative Research in Science and Engineering”, Amount: $4,600,351. Role: co-PI of 5 investigators, not PI. Term of award: 03/01/10 – 09/30/13.

National Science Foundation (CBET-0854340), “Modeling of fluids and interfaces via synthesis of integral equations and Mayer-sampling cluster integral calculations”, Amount: $300,000. Role: PI of 2 investigators. Term of award: 09/01/09 – 08/31/13.

National Science Foundation (CHE-0626305), “Collaborative Research: Cyberinfrastructure for Phase Space Mapping – Free Energies, Phase Equilibria, and Transition Paths”, Amount: $871,800. Role: Sole PI. Term of award: 10/01/06 – 09/30/12.

Petroleum Research Fund of the American Chemical Society, “Examination of the Role of Entropy and Defects on the Relative Stability of Molecular Crystals”, Amount: $100,000. Role: Sole PI. Term of Award: 01/01/08 – 08/31/11.

CACHE Corporation (NSF flow through (DUE-0618521), “CCLI: A Molecular Simulation Module Development Community, Amount: $241,952. Role: PI of 2 investigators. Term of award: 10/01/06 – 09/30/11.

University at Buffalo Interdisciplinary Research Development Fund, "Toward the first-principles calculation of bulk-phase thermophysical properties", Amount: $36,219. Term of award: 06/15/09 – 07/31/10.

National Science Foundation (CMMI-0508854), "Damage mechanics of nanoelectronics packaging solder joints", Amount: $284,500. Term of award: 08/01/05 – 07/31/09 (PI: C. Basaran).

IBM (Faculty Award for Innovation), "An extensible Eclipse-based application for molecular and mesoscale simulation", Amount: $22,500. Awarded 04/05.

National Science Foundation (CBET-0414439), "Mayer-sampling methods for calculation of statistical-mechanical cluster integrals: Nanotechnology and other applications", Amount: $300,000. Term of award: 06/01/04 – 03/31/08

National Science Foundation (CBET-0219266): "ITR: Advanced computational environment for molecular and mesoscale modeling", Amount: $499,128. Term of award: 09/01/02 – 08/31/07.

U.S. Department of Energy, "Studies of phase behavior and structure in solids", Amount: $335,000. Term of award: 06/01/03 – 08/31/07

National Science Foundation (DGE-0114330): "IGERT: Biophotonics Materials and Applications" Amount: $2,685,473. Term of award: 6/1/01-5/31/07. One of five co-PI's.

National Science Foundation (CBET-0423068), "2004 Midwest thermodynamics and statistical mechanics meeting", Amount: $7100. Term of award: 06/01/04 – 05/31/05. co-PI with J. Errington.

U.S. Department of Energy: "Molecular modeling of solid-phase thermodynamics, structure, and growth" Amount: $308,000. Term of award: 12/15/99 – 05/31/03.

National Science Foundation (CBET-0076515): "Development of high-quality models for anhydrous and aqueous hydrogen fluoride" Amount: $170,000. Term of award: 08/01/00 – 05/31/03.

National Science Foundation (DUE-9752243): "World-Wide-Web Based Modules for Introduction of Molecular Simulation into the Chemical Engineering Curriculum" Amount: $332,880. Term of award: 6/1/98 - 10/31/02. One of eleven Co-PI's from seven institutions.

National Science Foundation (CBET-9720705): "Development of High-Quality Molecular and Engineering Models for Hydrogen Fluoride and Its Mixtures" Amount: $155,003. Term of award: 3/1/98 - 5/31/01.

Petroleum Research Fund: "Understanding Insertion-Based Molecular Simulation Methods" Amount: $60,000. Term of award: 6/1/98 - 8/31/00.

U.S. Department of Education: "GAANN Fellowship Program: Environmentally Benign Chemical Processes and Products" Amount: $302,664. Term of award: 8/15/98 - 8/14/01. One of eight Co-PI's from SUNY Buffalo Department of Chemical Engineering.

National Science Foundation (EEC-9700809): "Development of a World-Wide-Web based textbook on molecular simulation: A dynamic approach to integrating fundamental concepts and research advances into the chemical engineering curriculum" Amount: $346,453. Term of award: 4/1/97 - 3/31/01. One of seven Co-PI's from seven institutions.

SUNY-Buffalo Multidisciplinary Research Pilot Project Program, "Theoretical Models of Hydrogen-Bonded Liquids" Amount: $20,000. Term of award: 6/1/99-12/31/00 (co-PI with Harry King of the UB Department of Chemistry).

U.S. Department of Energy: "Molecular simulation of phase coexistence, with application to ordered phases" Amount: $232,000. Term of award: 9/15/96 - 12/14/99

Petroleum Research Fund: "Construction of phase diagrams by molecular simulation, with application to intermolecular potential development" Amount: $50,000. Term of award: 7/1/96 - 8/31/98.

National Science Foundation (CBET- 9622204): "Engineering Research Equipment: High performance visualization hardware. Amount: $87,060 (including matching). Term of award: 6/1/96 - 5/31/97. One of three Co-PI's from SUNY Buffalo Department of Chemical Engineering.

Petroleum Research Fund: "Some new ideas for the treatment of conformal solutions" Amount: $50,000. Term of award: 7/1/94 - 8/31/96.

National Science Foundation (CBET-9057161): Presidential Young Investigator Award; Amount $25,000, + $37,500 matching for each of five years, 1990-1995.

National Science Foundation ILI-LLD: "Development of a Simulation Laboratory for Chemical Engineering Instruction" Amount: $97,251. (Co-PI's are S. Diamond, C. Lund, T. Mountziaris, J. Nitsche, M. Ryan, and T. Weber). Term of award: 7/1/93 - 6/30/95

Petroleum Research Fund: "A novel approach to conformal solutions" Amount: $40,000. Term of award: 6/1/91 - 8/31/94.

National Science Foundation (CBET-9212682): "Engineering research equipment: High-performance graphics workstation" Amount: $54,000. (Co-PI with T.J. Mountziaris, J.A. Tsonopoulos, and J.M. Nitsche).

Exxon Education Foundation, unrestricted grant. Amount: $10,000. Term of award: 10/1/91-5/30/93.

Pittsburgh Supercomputing Center: "Molecular thermodynamics and transport properties of model liquid-crystalline mixtures" Amount: 125 Cray units. Term of award: 1/15/92 - 1/15/93.

National Science Foundation (Initiation Grant) (CBET-8909365): "Molecular thermodynamics and transport properties of model liquid-crystalline mixtures" Amount: $70,000. Term of award: 9/1/89 - 5/31/92.

Pittsburgh Supercomputing Center: "Molecular thermodynamics and transport properties of model liquid-crystalline mixtures" Amount: 125 Cray units. Term of award: 10/1/90 - 1/15/92.

National Science Foundation (CBET-8912569): "Travel to the Fifth International Conference on Fluid Properties and Phase Equilibria for Chemical Process Design", Amount: $783. Term of award: 5/89.

Teaching Experience

Ph.D. Graduates

Arpit Bansal, 2022, "Methods to Evaluate Virial Coefficients from Molecular Models", Subsequently employed by a start-up company in India.

Navneeth Gokul, 2021, "Accurate Thermodynamic Properties of Fluids from Molecular Models via the Virial Equation of State." Subsequently at postdoc at the University of Rochester.

Weisong Lin, 2019, "Mapped Averaging for Molecular Rotation." Subsequently employed by M&T Bank.

Apoorva Purohit, 2019, "Mapped Averaging Methods for Highly Efficient Evaluation of Thermodynamic Properties. Subsequently a postdoc at Los Alamos National Laboratory.

Shu Yang, 2016, *"*Molecular-Based Modeling of Gases and Gaseous Mixtures via the Virial Equation of State."

Chao Feng, 2016, *"*Techniques for Computing High-Order Virial Coefficients Using Mixed-Precision Approach for Hybrid Architectures" (co-advised CSE student).

Ramachandran Subramanian, 2016, "Quantum Virial Coefficients via Path Integral Monte Carlo: Theory and Development of Novel Algorithms." Subsequently at postdoc at University at Buffalo (Computer Science).

Sabry G. Moustafa, 2015, "Efficient Molecular Simulation Methods for Evaluation of Thermodynamic Properties of Crystalline Phases." Subsequently a postdoc at University at Buffalo.

Jung Ho Yang, 2015, "Molecular Modeling Based on Statistical Mechanics for Inhomogeneous Fluids." Subsequently at postdoc at Drexel University.

Hye Min Kim, 2011, "A Virial Equation of State of Associating Systems Based on Wertheim's Association Theory."

Katherine R. Shaul, 2011, "Monte Carlo Methods for the Development of *Ab Initio* Virial Equations of State."

Tai Boon Tan, 2011, "Novel Methods for Solid-State Free-Energy Calculations", subsequently employed by General Physics Corp.

Michael S. Sellers, 2010, "Atomistic Modeling of the Microstructure and Transport Properties of Lead-Free Solder Alloys," subsequently a postdoc at the U.S. Army Research Laboratory.

Di Wu, 2005, "Development and Application of Phase-Space Overlap Measures for Free-Energy Calculations," subsequently a postdoc at the University of California at Berkeley.

Sang Kyu Kwak, 2005, "Studies of Point Defects in Strained Solids by Molecular Simulation," subsequently an Assistant Professor at the Nanyang Technological University, Singapore.

Jayant Singh, 2005, "Molecular Simulation Study of Fundamental Effects of Molecular Association on Properties of Fluid Interfaces," subsequently and Assistant Professor at IIT Kanpur.
Jhumpa Adhikari, 2003, "Free Energy and Phase Equilibria of Solids by Molecular Simulation," subsequently an Assistant Professor at IIT Bombay.
Scott J. Wierzchowski, 2003, "Molecular Models for Hydrogen Fluoride," subsequently a postdoc at the University of Massachusetts.
Nandou Lu, 2002, "Accuracy and Precision of Free-energy Calculations via Molecular Simulation," subsequently a postdoc at Johns Hopkins University.
C. Daniel Barnes, 2001, "Computer Simulation of Solid-Phase Equilibria," subsequently employed by Westinghouse.
Donald P. Visco, Jr., 1999, "Thermodynamic and Molecular Modeling of Hydrogen Fluoride," subsequently an Assistant Professor at Tennessee Technological University.
Anjali A. Khare, 1997, "Molecular Modeling of Liquid Crystals. Molecular Simulations and Statistical Mechanical Theories," subsequently a postdoctoral associate with Gregory Rutledge of MIT.
Durgesh S. Vaidya, 1997, "Convection-Diffusion of Solutes in Dynamic Media: Application to Electrophoretic Separation Using Liquid Crystalline Materials," subsequently employed by SpecTran Corporation.
Manoj Mehta, 1996, "Computer Simulation of Multi-phase Equilibria," subsequently employed by Ford Motor Company, Inc.
Hung-chang Chiu, 1995, "New Approaches to Conformal Solutions," subsequently employed by IntePlast, Inc.
Rupal Agrawal, 1995, "Molecular Simulation of Solid-Fluid Phase Coexistence," subsequently a Postdoctoral Associate at Argonne National Laboratory

M.S. Graduates

Sykhere Brown, 2022, "Performance of mapped averaging in computing the elastic properties of soft-sphere crystals."
Pavan Behara, 2014, "Additive binary hard-sphere mixtures: Eighth-order virial equation of state and stability analysis."
Saranya Harikrishnan, 2011, "Calculation of virial coefficients using Mixture Builder," subsequently employed by AspenTech.
Srihari Gangaikondan Sankararaman, 2011, "Implementation of fast Fourier transforms and integral equation theories towards calculating virial coefficients," subsequently employed by Velcro USA.
Venkata Suryanarayana Murthy Josyula, 2011, "Virial coefficients and equations of state for Malescio-Pellicane and Gaussian-core potential models," subsequently employed by GEA PHE Systems.
Bryan Mihalick, 2001, "Development of a Standalone Java-Based Molecular Simulation Environment," subsequently employed by IBM.
Edhi Juwono, 1999, "Engineering modeling of hydrogen fluoride and water mixtures using the statistical associating fluid theory," subsequently employed by Texaco.
Jeffrey Aaron Henning, 1998, "Efficient evaluation of bubble-dew and residue curves via molecular simulation," subsequently employed by Graham Manufacturing.
Sandeep P. Pandit, 1998, "Efficient methods for calculating bubble-dew and azeotrope curves by molecular simulation," subsequently employed by SpecTran Corporation.
Clifford J. Post, 1994, "Modeling of Inhomogeneous Fluids by Hard Disks in a Finite Periodic Narrow Box," concurrently employed by Iimac, Inc.

M.S. Graduates (non-thesis)

Nancy Cribbin
Fan Zhang

M.E. Graduates

Siren Tang
Akshara Goyal

Former Postdoctoral Fellows

Kenneth Benjamin, Object-oriented software development; Application of Mayer-sampling methods; subsequently an Assistant Professor at South Dakota School of Mines.
Nate Barlow, Analysis of convergence of virial and other cluster series; parallel computation methods; subsequently an Assistant Professor at Rochester Institute of Technology.
Fenglai Liu, Density functional theory methods for *ab initio* energy calculations
Sabry Gad Al Hak Moustafa, Free energy and phase equilibria methods for solids

Current Postdoctoral Fellows/Research Assistants

Andrew Schultz (Research Associate Professor), Object-oriented software development; Development of Mayer-sampling methods; Free energy methods for solids

Current Ph.D. Students

Omkar Desai, Molecular modeling of membrane separations

Current M.S. Students

None

Current M.E. Students

None

Courses Taught

ChE 100 *Introduction to Chemical Engineering*; Fall 1986 (instructor at U. Penn).
EAS 140 *Introduction to Engineering*; Fall 1995, 1997, 2006.
EAS 230 *Engineering Computations*; Fall 2007-09.
CE 212 *Introduction to Chemical Engineering*; Fall 1989-95.
CE 304 *Chemical Engineering Thermodynamics*; Spring 1998-99.
CE 317 *Transport Phenomena I*; Fall 1997-99, Fall 2001-03, Fall 2005-07, Fall 2009-10.
CE 327 *Chemical Engineering Lab I: Probability, Statistics, and Data Analysis*; Fall 2012-21.
CE 341 *Applied Mathematics for Chemical Engineers*; Fall 2020-23.
CE 400 *Honors Seminar on Molecular Simulation*; Fall 2001.
CE 412 *Molecular Modeling* (co-taught with J. Errington); Spring 2004, 2005.
CE 427 *Chemical Engineering Lab 3*; Fall 1990.

CE 525 *Advanced Chemical Engineering Thermodynamics*; Spring 1990-91, Fall 1991-95, Spring 1998, 2000-02.
CE 498 *Undergraduate Research*; Fall 2014-15; Spring-Fall 2015-18.
CE 526 *Statistical Mechanics*; Spring 1992-93, 1995, 1999, 2004, 2013; Fall 2000, 2005.
CE 530 *Molecular Simulation*; Spring 2000, 2003, 2014, 2016, 2017.

Other Experience

- Co-PI on two NSF funded projects to develop computer-based instructional media for teaching molecular concepts in chemical engineering.
- Supervised numerous undergraduate and graduate students in independent research projects

Service to the University

Director of Undergraduate Studies, Dept. of Chemical & Biological Engineering; 1991-96, 1997-2006, 2018-.
Chair, CBE Teaching Faculty Search Committee, 2022-23.
Member, SEAS JEDI (Justice, Equity, Diversity, Inclusion) Task Force
Co-facilitator, Summer SEAS Instructional Excellence Working Group, 2020-21.
Chair, CBE Faculty Search Committee, 2019-20.
Member, SEAS Dean Search Committee, 2019-20.
Co-organized inaugural Chemical Engineering Summer Camp, July 22-26, 2019.
Chair, Jacobs School of Medicine and Biomedical Sciences Decanal Review Committee, 2016-17.
Co-Chair, CBE Awards Committee, 2012-
Member, School of Dental Medicine Decanal Review Committee, 2014-15.
Member, Provost's Excellence in Scholarship and Creative Activities Committee, 2013-
Chair, CBE Faculty Search Committee, 2012-13.
Director of Computational Science and Information Technology, CBE, 2012-
Member, Davis Hall landscaping committee, 2010-11.
Co-Chair, Department of Biomedical Engineering; 2010-2012.
Chair, Department of Chemical and Biological Engineering; 2006-2012.
Member, SEAS Communication Specialist Search Committee; Spring 2008.
Member of Chemical Engineering Undergraduate Committee; 1989-2006, 2012-present.
Member, University academic integrity standing committee, 2003-04.
Chair, Provost's *ad hoc* Research Advisory Committee for SEAS, 2002-03.
Member, Provost's *ad hoc* advisory committee for CCR, 2003.
Member, SEAS Faculty Personnel Committee, 1998-2000, 2001-05; Chair 1999-2000.
Chair, SEAS Decanal Review Committee, 2002.
Educational Technology grant review panel, 2001.
Member, *ad hoc* grievance committee, March 2000.
Member, *ad hoc* committee on MTH 417, 418, 445, 449, Fall 1999.
Member, Technical Communications Steering Committee, 1999-present.
Chair, Scientific Board, UB Center for Computational Research, 1999-present.
Chair, User Advisory Board, UB Center for Computational Research, 1999.
Educational Technology grant review panel, 1999.
Creation and maintenance of Chemical Engineering Department web site 1998-present.
Member of FNSM/SEAS Learning, Teaching, Technology Roundtable, 1997-98.
Member of Provost's *ad hoc* committee for high-performance research computing, 1998.

SEAS representative on the Committee on Math 306, 1995-96
Member of faculty search committee, Department of Chemical Engineering; 1995-96, 98-99, 2000.
Member of the *ad hoc* committee to review computing instruction; 1994-95Supervised Chemical Engineering Industrial Internship Program; 1990-91
Produced Chemical Engineering Graduate Brochure; 1991
Served on Chairman Search Committee of the Department of Chemical Engineering; 1990

Professional Activities

Editorial

Associate Editor, *Journal of Chemical & Engineering Data*, 2016-.
Guest Editor, *Molecular Physics*, special issue in honor of Peter T. Cummings, 2019.
Member of Editorial Board of *Molecular Physics*, 2007-.
Member of Editorial Advisory Board of *Journal of Chemical & Engineering Data*, 2013-2015.

Boards

Advisory Board, Department of Chemical and Biomedical Engineering, Rochester Institute of Technology, 2011-2023.

Symposium Chair

1. "In Honor of Peter Monson", AIChE Annual Meeting, Pittsburgh, PA; October 2018.
2. "CACHE Symposium: Honoring Award Recipients", AIChE Annual Meeting, Salt Lake City, UT; November 2010.
3. "Symposium honoring CAChE award recipients", AIChE Annual Meeting, Nashville, TN; November 2009.
4. "Statistics and Sampling", Computational Chemistry Gordon Conference – New Computational Tools for the 21st Century; Mount Holyoke College, South Hadley, MA; July 2008.
5. "20 Years of the Gibbs Ensemble", AIChE Annual Meeting, Salt Lake City, UT; November 2007.
6. "Teaching Molecular Simulation", AIChE Annual Meeting, Austin, TX; November 2004.
7. "Thermodynamics of Solid-Fluid Phase Equilibria", AIChE Annual Meeting, Indianapolis, IN; November 2002.
8. "Thermodynamics of Solid-Fluid Phase Equilibria", AIChE Annual Meeting, Reno, NV; November 2001.
9. "Poster Session: Thermodynamics and Transport Properties", AIChE Annual Meeting, Los Angeles, CA; November 2000.
10. "Molecular Simulation Methods and Force field Development", AIChE Annual Meeting, Dallas, TX; November 1999.
11. "Solid-Fluid Phase Transitions: Thermodynamics and Kinetics", AIChE Annual Meeting, Miami Beach, FL; November 1998.
12. "Thermodynamic Properties and Phase Behavior: General", AIChE Annual Meeting, Los Angeles, CA; November 1997.

13. "Thermodynamic Properties and Phase Behavior: Simulation", AIChE Annual Meeting, Chicago, IL; November 1996.
14. "Fundamentals of Solid-Fluid Equilibrium", AIChE Annual Meeting, Miami Beach, FL; November 1995.
15. "Molecular Simulation and Theory of Thermophysical Properties," AIChE Annual Meeting, San Francisco, CA; November 1994.
16. "Thermodynamics and Transport Properties in Structured Polymers Liquids and Gels," AIChE Annual Meeting, Los Angeles, CA; November 1991.
17. "Microscopic and Molecular-Based Models," AIChE Annual Meeting, Chicago, IL; November 1990.

Professional Committee Memberships

CACHE (Computer Aids for Chemical Engineering) Board of Trustees, 1999-2022; Secretary 2004-2006; Vice President, 2008-2010; President 2010-2012; Advisor 2023-present.
CACHE (Computer Aids for Chemical Engineering) Task Force on Molecular Modeling, 1996-present.
International Program Committee for the Third International Conference on the Foundations of Molecular Modeling and Simulation (FOMMS)
Member, AIChE Computational Molecular Science and Engineering Forum (CoMSEF), 2001-present; Vice-Chair for Membership, 2007-present.
Member, AIChE Nanoscale Science and Engineering Forum
Area 1a Programming Chair for the Annual Meeting of the AIChE, Los Angeles, November 2000.
Area 1a (Thermodynamics and Transport Properties) of the AIChE, 1996-2002.
Engineering and Physical Sciences Research Council (EPSRC) Peer Review College, 2006-09.

Professional Society Memberships

Fellow, American Institute of Chemical Engineers. Member, 1990-2007; Senior Member, 2007-2014.
Fellow, American Association for the Advancement of Science.
Member, American Chemical Society, 1989-present.
Member, Materials Research Society.
Member, American Geophysical Union.
Member, American Society for Engineering Education

Workshop Participation

1. ACS Leading Inclusively Course on Diversity, Equity, Inclusion, and Respect, June 2021.
2. MolSSI Workshop for Best Practices in Molecular Simulation, Gaithersburg, MD; August 2017.
3. Atomistic Simulations for Industrial Needs Workshop, National Institute of Standards & Technology (NIST), Gaithersburg, MD; August 2013.
4. CECAM – New Directions in Liquid State Theory, Lyon, France; July 2007.
5. SimBioMa Workshop on Sampling Paths in Molecular Simulation: Algorithms for Phase Transitions, Reactivity, and Kinetics; Orsay, France; November 2006.

6. NSF Workshop on Cyberinfrastructure in Chemical and Biological Systems; Arlington, VA; September 2006.
7. Industrial Fluid Properties Simulation Collective (IFPSC) Workshop; St. Paul, MN; September 2006.
8. NSF Workshop on Cyber-enabled Chemistry; Arlington, VA; October 2004.
9. CECAM – Continuing Challenges in Free Energy Calculations: Theory and Applications in Chemistry and Biology, Lyon, France; May 2004.
10. CECAM – Modeling Crystallization and Stability of Organic Solids, Lyon, France; May 2003.
11. German-American Frontiers of Engineering, sponsored by the National Academy of Engineering and the Alexander von Humboldt Foundation, Ludwigsburg, Germany; May 2003.
12. NIST – Predicting Thermophysical Properties; Gaithersburg, MD; June 2001.
13. Frontiers of Engineering, sponsored by the National Academy of Engineering, Irvine, CA; May 2001.
14. CECAM – Algorithms for Simulating Complex Molecular Systems, Lyon, France; May 1998.
15. U.S. Department of Energy, Council on Chemical Sciences Workshop – Research Frontiers in Molecular Simulation and Computational Chemistry: Extending the Accuracy and Scale of Molecular-Based Calculations; Santa Fe, NM; May 1998.
16. U.S. Department of Energy, Office of Industrial Technologies – Computational Chemistry Technology Roadmap Workshop: Design of a Chemical System with Targeted Properties; College Park, MD; March 1998.
17. U.S. National Science Foundation –Workshop on Molecular Modeling and Simulation: Fundamentals and Applications; Arlington, VA; November 1997.
18. CECAM – Development of Transferable Intermolecular Potentials for Phase Equilibria Calculations, Lyon, France; May 1996.

Workshops Conducted

1. D.A. Kofke, “Introduction to Molecular Simulations, Ensembles, and Connection to Thermodynamics” (Parts 1 and 2); “Introduction to Monte Carlo Simulations”; “Introduction to Free Energy Calculations”, *Fundamentals of Molecular Simulation 2020*, IIT Kanpur, India; February 2020.
2. D.A. Kofke and A.J. Schultz, “Molecular Simulation Modules” (2 sessions), ASEE Chemical Engineering Summer School, Raleigh, NC; July 2017.
3. D.A. Kofke and A.J. Schultz, “Quantifying uncertainty in molecular simulations”, AIChE Annual Meeting, Minneapolis, MN; October 2017.
4. D.A. Kofke and A.J. Schultz, “Open-source molecular simulation standards”, FOMMS 2009, Semiahmoo Resort, Blaine, WA; July 2009.
5. D.A. Kofke and A.J. Schultz, “Molecular simulation modules”, FOMMS 2009, Semiahmoo Resort, Blaine, WA; July 2009.
6. D.A. Kofke and P.T. Cummings, “Teaching Molecular Simulation”, ASEE Chemical Engineering Summer School, Pullman, WA; August 2007.
7. D. A. Kofke, “Web-based technologies for teaching and using molecular simulation”, PPEPPD Conference, Kurashiki, Japan; May 2001.

Conferences Organized

Co-Chair, Sixth International Conference on Foundations of Molecular Modeling and Simulation (FOMMS) 2015.
Midwest Thermodynamics and Statistical Mechanics Conference, held on the University at Buffalo campus on June 3-4, 2004. (co-organized with J.R. Errington).

Presentations

Invited

1. D.A. Kofke, "The virial equation of state merits more attention", CECAM Workshop on "Challenges and opportunities in nonequilibrium soft matter" on the occasion of the 75th birthday of Daan Frenkel, Mont Sant Benet, Spain; September 2023.
2. D.A. Kofke, "On the activity virial series", Symposium honoring Pablo Debenedetti on his 70th birthday, Princeton University, Princeton, NJ; June 2023.
3. D.A. Kofke, "Origins of the failure of the activity virial series", Symposium honoring Keith Gubbins, Heriot-Watt University, Edinburgh, Scotland; May 2023.
4. D.A. Kofke, "Bridging molecular and thermodynamic properties using cluster integrals and the virial equation of state", Applied Thermodynamics and Molecular Simulation (ATOMS) Online Seminar; June 2022.
5. D.A. Kofke, "The 'Easy' Thermodynamic Phases Can Provide Interest, Challenge, and Opportunity", Department of Chemical Engineering, Rochester Institute of Technology, Rochester, NY; February 2022.
6. D.A. Kofke, "Keynote Lecture: The Role of Molecular Modeling in Applied Thermodynamics", Thermodynamik-Kolloquium 2021, Online event hosted in Germany, September 2021.
7. D.A. Kofke, "The 'Easy' Thermodynamic Phases Can Provide Interest, Challenge, and Opportunity", Department of Chemistry, University of Kansas, Lawrence, KS, April 2021.
8. D.A. Kofke, "Mapped Averaging Methods for Deriving Ensemble Averages: Application to Crystals", Symposium on Molecular Simulations of Complex Fluids and Interfaces, IIT Kanpur, India; February 2020.
9. David A. Kofke, Sabry G. Moustafa, Andrew J. Schultz, Francis W. Starr and Jack F. Douglas, "Quantify dynamic heterogeneity of glasses: Percolation perspective", Session on *Thermodynamics at the NanoScale*, AIChE Annual Meeting, Orlando, FL; November 2019.
10. D.A. Kofke, "Computational cluster-integral methods for solutions", session on *Interactions of Macromolecules, Ions and Colloids in the Condensed Phase: Computational and Experimental Advances* at the Canadian Society for Chemistry Conference, Quebec City; June, 2019.
11. D.A. Kofke, "Cluster-integral methods for prediction of fluid-phase properties from molecular models", 15th International Conference on Properties and Phase Equilibria for Products and Process Design (PPEPPD 2019), Vancouver, Canada.
12. D.A. Kofke, "The 'Easy' Phases Can Still Provide Interest, Challenge, and Opportunity", Chinese Thermophysical Properties Conference, Hanzhong, China; October 2018

13. Sabry G. Moustafa, Andrew J. Schultz, Eva Zurek, and David A. Kofke, "Crystal Structure of Iron at High Temperature and Pressure", 20th Symposium on Thermophysical Properties, Boulder, CO; June 2018.
14. D.A. Kofke, "The 'Easy' Phases Can Still Provide Interest, Challenge, and Opportunity", National Institute of Standards and Technology (NIST), Gaithersburg, MD; May 2018.
15. D.A. Kofke, "The 'Easy' Phases Can Still Provide Interest, Challenge, and Opportunity", Department of Chemical Engineering, Yale University, New Haven, CT; April 2018.
16. D.A. Kofke, "The 'Easy' Phases Can Still Provide Interest, Challenge, and Opportunity", Department of Chemical Engineering, University of New Hampshire, Durham, NH; April 2018.
17. A.J. Schultz, S.G. Moustafa, and D.A. Kofke, "Harmonically mapped averaging for direct evaluation of anharmonic properties of solids by molecular simulation", CECAM workshop on "Anharmonicity and thermal properties of solids, Institut Henri-Poincaré, Paris, France; January 2018.
18. D.A. Kofke, "Computational cluster-based methods for molecular thermodynamics", Workshop on "Fundamental theoretical approaches to the equation of state", University of Manchester, Manchester, UK, January 2018.
19. D.A. Kofke, "The 'Easy' Phases Can Still Provide Interest, Challenge, and Opportunity", Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC; October 2017.
20. D.A. Kofke, "Mapped averaging methods for high-precision, high-efficiency calculation of properties by molecular simulation", Ulam Computer Simulations Workshop, Lviv, Ukraine; June 2017.
21. D.A. Kofke, "The 'Easy' Phases Can Still Provide Interest, Challenge, and Opportunity", Department of Chemical Engineering, University of Rochester, Rochester, NY; March 2017.
22. D.A. Kofke, "The 'Easy' Phases Can Still Provide Interest, Challenge, and Opportunity", Department of Chemistry, University of Western Ontario, London, ON; February 2017.
23. D.A. Kofke, "Big Properties from Small Simulations", Department of Chemical Engineering, Rochester Institute of Technology, September 2015.
24. S.G. Moustafa, A.J. Schultz, and D.A. Kofke, "Very Efficient Methods for Evaluation of Properties of Crystalline Phases by Molecular Simulation", Nineteenth Symposium on Thermophysical Properties, Boulder, CO; June 2015.
25. D.A. Kofke, "Big Properties from Small Simulations", Department of Chemical Engineering, Case Western Reserve University, March 2015.
26. D.A. Kofke, "Computational Cluster-Based Methods for Molecular Thermodynamics", AIChE Annual Meeting, Session in honor of Peter Cummings, Atlanta, GA; November 2014.
27. D.A. Kofke, "Big Properties from Small Simulations", School of Engineering and Applied Sciences, University of Manchester, Manchester, UK; June 2014.
28. D.A. Kofke, "Series-Based Methods for Associating Fluids", *SAFT 2014: From SAFT to Experiment and Back*, Tróia, Portugal; April 2014.
29. D.A. Kofke, "Recent Advances in the Calculation and Application of Virial Coefficients and Cluster Integrals", New York Theoretical and Computational Chemistry Conference (NYTaC^3), City University of New York, New York, NY; January 2013.

30. D.A. Kofke and A.J. Schultz, Himmelblau Award Lecture, AIChE Annual Meeting, Pittsburgh, PA; October 2012.
31. D.A. Kofke, "Big Properties from Small Simulations", Department of Chemical Engineering, University of Akron, October 2012.
32. D.A. Kofke, "On Bias in Free Energy Calculations, and Some Free-Energy Methods for Crystalline Phases", CECAM workshop on *Free Energy Calculations: From Theory to Application*, Ecole des Ponts, Champs-sur-Marne, France; June 2012.
33. D.A. Kofke, "Big Properties from Small Simulations", Center for Research Computing, University of Notre Dame, April 2012.
34. D.A. Kofke, "Some Recent Advances in Free Energy and Sampling Methods for Crystals, Mixtures and Coexisting Phases", Navigating Chemical Compound Space for Materials and Bio Design. Workshop IV: Physical Frameworks for Sampling Chemical Compound Space, Institute of Pure and Applied Mathematics, UCLA, Los Angeles, CA; May 2011.
35. D.A. Kofke and A.J. Schultz, "Molecular simulation modules for instruction in thermodynamics, transport, kinetics, and materials", ASEE St. Lawrence Section 2011 Conference, *Innovations in Engineering and Technology Education*; March 2011.
36. D.A. Kofke, "Big Properties from Small Simulations", Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA; January 2010.
37. D.A. Kofke, "The 'Easy' Phases Can Still Provide Interest, Challenge, and Opportunity", Department of Chemical Engineering, Texas A&M University, College Station, TX; March 2009.
38. D.A. Kofke, "The 'Easy' Phases Can Still Provide Interest, Challenge, and Opportunity", *Schlumberger Lecture, D.B. Robinson Distinguished Speaker Series*, Department of Chemical and Materials Engineering, University of Alberta, Edmonton, Alberta; February 2009.
39. D.A. Kofke, "Molecular Concepts in Thermodynamics Education", Topical Conference on *A Century of Chemical Engineering Thermodynamics Education*, AIChE Annual Meeting, Philadelphia, PA; November 2008.
40. D.A. Kofke, "Good + Bad = Ugly, and other pitfalls to avoid when calculating free energies," Department of Chemical Engineering, Rensselaer Polytechnic University, Troy, NY; November 2008.
41. D.A. Kofke, "Good + Bad = Ugly, and other pitfalls to avoid when calculating free energies," Department of Chemical Engineering, University of Rhode Island, Kingston, RI; September 2008.
42. D.A. Kofke, "Statistics and Sampling", Computational Chemistry Gordon Conference – New Computational Tools for the 21st Century; Mount Holyoke College, South Hadley, MA; July 2008.
43. D.A. Kofke, "Fail-safe Bias Detection and Design of Stages through Consideration of Phase-space Overlap", Workshop on *Mathematical and Numerical Methods for Free Energy Calculations in Molecular Systems*, Banff International Research Station (BIRS) for Mathematical Innovation and Discovery, Banff, Alberta, Canada; June 2008.
44. D.A. Kofke, "Good + Bad = Ugly, and other pitfalls to avoid when calculating free energies," Department of Chemical Engineering, Brigham Young University, Salt Lake City, UT; April 2008.
45. D.A. Kofke, "Good + Bad = Ugly, and other pitfalls to avoid when calculating free energies," *2008 Johansen-Crosby Lecture in Chemical Engineering*, Michigan State University, East Lansing, MI; March 2008.

46. D.A. Kofke, "A molecular simulation module-development community," *2008 Johansen-Crosby Lecture in Chemical Engineering*, Michigan State University, East Lansing, MI; March 2008.
47. D.A. Kofke, "Good + Bad = Ugly, and other pitfalls to avoid when calculating free energies", Department of Chemical Engineering, Case-Western Reserve University, Cleveland, OH; March 2008.
48. D.A. Kofke, "Area 1a Keynote Address: The "Easy" Phases Can Still Provide Interest, Challenge, and Opportunity", AIChE Annual Meeting, Salt Lake City, UT; November 2007.
49. D.A. Kofke, "Molecular modeling and simulation" (Schoellkopf Award Lecture), Western New York ACS chapter meeting, Buffalo, NY; September 2007.
50. D.A. Kofke, "Optimal evaluation of free energies by molecular simulation", Second International Conference on Continuous Optimization + Modeling and Optimization: Theory and Applications, McMaster University, Hamilton, ON; August 2007.
51. A.J. Schultz, K.M. Benjamin, and D.A. Kofke, "Advances in the Numerical Calculation of Virial Coefficients", CECAM Workshop: *New Directions in Liquid State Theory*, Lyon, France; July 2007.
52. D.A. Kofke, "Good + Bad = Ugly, and other pitfalls to avoid when calculating free energies", Department of Chemical Engineering, University of Texas, Austin, TX; April 2007.
53. D.A. Kofke, J.R. Errington, and A.J. Schultz, "Progress in developing a web-based database-driven curriculum assessment tool", 233rd ACS National Meeting, Chicago, IL; March 2007.
54. D.A. Kofke, "Generation of transition paths and calculation of free energies using Rosenbluth sampling", SimBioMa Workshop on Sampling Paths in Molecular Simulation: Algorithms for Phase Transitions, Reactivity, and Kinetics; Orsay, France; November 2006
55. D.A. Kofke, "Advances in Evaluation of Free Energy and Other Configurational Integrals by Molecular Simulation", Seventh Liblice Conference on the Statistical Mechanics of Liquids, Lednice, Czech Republic, June 2006.
56. D.A. Kofke, "Etomica: An API for Molecular Simulation", Oak Ridge National Laboratory, May 2005.
57. D.A. Kofke, "Making room for intuition in molecular simulation", Sessions honoring Eli Ruckenstein on his 80th birthday, AIChE Annual Meeting, Cincinnati, OH, November 2005.
58. D.A. Kofke, "Free energy and all that", Department of Chemical Engineering, Iowa State University, Ames, IA; October 2004.
59. D.A. Kofke "Free energy and all that" Tenth International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Snowbird, UT; May 2004.
60. D.A. Kofke, "Thinking about phase-space overlap to guide the implementation of free energy calculations", CECAM Workshop: *Continuing challenges in free energy calculations: Theory and applications in chemistry and biology*, Lyon, France; May 2004.
61. D.A. Kofke, "Free energy and all that", Department of Chemical Engineering, Ohio State University, Columbus, OH; April 2004.
62. D.A. Kofke, "Free energy and all that", Department of Chemical Engineering, Vanderbilt University, Nashville, TN; February 2004.
63. D.A. Kofke, "Getting the most from molecular simulation", Department of Chemical Engineering, Colorado State University, Fort Collins, CO; October 2003.
64. D.A. Kofke, "Getting the most from molecular simulation", Department of Chemical Engineering, Colorado School of Mines, Golden, CO; October 2003.
65. D.A. Kofke, "Getting the most from molecular simulation", Department of Chemical Engineering, University of Michigan, Ann Arbor, MI; September 2003.

66. D.A. Kofke and J.K. Singh, "Effect of molecular association on vapor-liquid surface tension", 226th National Meeting of the ACS, New York, NY; September 2003.
67. D.A. Kofke, "Getting the most from molecular simulation", Foundations of Molecular Modeling and Simulation (FOMMS), Breckenridge, CO; July 2003.
68. D.A. Kofke, "Attempts to develop a direct method for evaluation of solid-phase free energies by molecular simulation", CECAM Workshop: *Modeling Crystallization and Stability of Organic Solids*, Lyon, France; May 2003.
69. D.A. Kofke, "Understanding thermodynamics with molecular simulation (and vice versa)", Department of Chemical Engineering, Texas A&M University, College Station, TX; March 2003.
70. D.A. Kofke, "Understanding thermodynamics with molecular simulation (and vice versa)", Department of Chemical Engineering, Georgia Institute of Technology; Atlanta, GA; November 2002.
71. N. Lu and D. A. Kofke, "Good + bad = bad: Forward and reverse FEP calculations should not be averaged ", 224th ACS National Meeting, Boston, MA; August 2002.
72. D.A. Kofke, "Understanding thermodynamics with molecular simulation (and vice versa)", Department of Chemical Engineering, Clarkson University; April 2002.
73. D.A. Kofke, "Understanding thermodynamics with molecular simulation (and vice versa)", Department of Chemical Engineering, University of California, Los Angeles; February 2002.
74. D.A. Kofke, "Molecular modeling and applications of phase transitions in solids", 76th International Bunsen Discussion Meeting: Global Phase Diagrams. Walberberg, Germany, August, 2001.
75. D.A. Kofke, "Appropriate and effective measurement of free energies", NIST Workshop on Predicting the Thermophysical Properties of Fluids by Molecular Simulation, Gaithersburg, MD; June 2001.
76. D.A Kofke, "Web-based technologies for teaching and using molecular simulation", Conference on Physical Properties and Phase Equilibria for Product and Process Design. Kurashiki, Japan, May 2001.
77. "Understanding Thermodynamics via Molecular Simulation (and vice versa)," Department of Chemical Engineering, University of Rochester, April 2001.
78. "Understanding Thermodynamics via Molecular Simulation (and vice versa)," Department of Chemical Engineering, University of Washington, April 2001.
79. "Advances in the Understanding and Application of Molecular Simulation", Department of Chemistry, Duquesne University, October 1999.
80. "The Role of Molecular Simulation in Chemical Engineering", Department of Chemical Engineering, Tohoku University, Sendai, Japan, September 1999.
81. "Improvements in the Understanding and Application of Molecular Simulation", AIChE-SCEJ Joint Symposium on Molecular Modeling, SCEJ Autumn Meeting, Kanazawa, Japan, September 1999.
82. "The Role of Molecular Simulation in Chemical Engineering", Department of Chemical Engineering, McMaster University, March 1999.
83. "Understanding Insertion-Based Molecular Simulation Techniques", Fifth Liblice Conference on the Statistical Mechanics of Liquids, Zelezna Ruda, Czech Republic; June 1998.
84. "Modeling Free-Energy Calculations", CECAM Workshop on Algorithms for Simulating Complex Molecular Systems, Lyon, France; May 1998.
85. "Solid-Fluid Coexistence for Polydisperse Hard Spheres", XXVII Winter Meeting on Statistical Physics, Cuernavaca, Mexico; January 1998.

86. "A World-Wide-Web Based Textbook on Molecular Simulation", ASEE Summer School for Chemical Engineering Faculty, Snowbird, UT; August 1997 (with P.T. Cummings).
87. "Efficient and Robust Evaluation of Thermodynamic Phase Diagrams by Molecular Simulation", Department of Chemistry, University of Minnesota; October, 1996.
88. "Efficient and Robust Evaluation of Thermodynamic Phase Diagrams by Molecular Simulation", Department of Chemical Engineering, University of Wisconsin; October, 1996.
89. "Efficient and Robust Evaluation of Phase Diagrams by Molecular Simulation", Department of Chemical Engineering, University of Tennessee; March 1995.
90. "Numerical Methods and Molecular Simulation", CCP5 Spring School on Methods in Molecular Simulation, Southampton University, United Kingdom; March 1995.
91. "Efficient and Robust Evaluation of Phase Diagrams by Molecular Simulation", Department of Physics, State University of New York at Buffalo; February 1995.
92. "Efficient and Robust Evaluation of Phase Diagrams by Molecular Simulation", Department of Chemical Engineering, University of Notre Dame; December 1994.
93. "A New Look at Conformal Solutions", Department of Chemical Engineering, University of Massachusetts; November 1993.
94. "A New Look at Conformal Solutions", Department of Chemical Engineering, State University of New York at Buffalo, October 1993.
95. "A New Look at Conformal Solutions", Department of Chemical Engineering, University of Pennsylvania; April 1993.
96. "A New Look at Conformal Solutions", School of Chemical Engineering, Cornell University; February 1993.
97. "Dimensional Reduction and Conformal Solutions: The 1-1/2 Fluid Theory", Department of Physics, State University of New York at Buffalo, Buffalo, NY; March 1992.
98. "Dimensional Reduction and Conformal Solutions: The 1-1/2 Fluid Theory", Department of Chemistry, University of Toronto, Toronto, Canada; March 1992.
99. "The Role of Molecular Simulation in Chemical Engineering", Department of Chemical Engineering, Purdue University, West Lafayette, IN; May 1988.
100. "The Role of Molecular Simulation in Chemical Engineering", Department of Chemical Engineering, Rice University, Houston, TX; April 1988.
101. "The Role of Molecular Simulation in Chemical Engineering", Department of Chemical Engineering Department, State University of New York at Buffalo, Buffalo, NY; February 1988.

Contributed (underline indicates speaker)

1. Andrew Schultz and David A. Kofke, "Volume-dependent virial coefficients", AIChE Annual Meeting, Orlando, FL; November 2023.
2. Sabry Moustafa, Andrew J. Schultz, and David A. Kofke, "Efficient Measurement of Anharmonic Mechanical Properties of Crystals Using Normal-Mode Mapping", AIChE Annual Meeting, Boston, MA; November 2021.
3. Arpit Bansal, Andrew J. Schultz, David A. Kofke, "Evaluation of Osmotic Virial Coefficients with Support from Gas-Phase Mixture Coefficients", AIChE Annual Meeting, Boston, MA; November 2021.
4. Arpit Bansal, Andrew J. Schultz, David A. Kofke and Jack F. Douglas, "A Software Module for Calculation of Virial Coefficients of Macromolecules", AIChE Annual Meeting, Orlando, FL; November 2019.

5. Navneeth Gokul, Andrew J. Schultz and David A. Kofke, "Experimental Validation of 2- and 3-Body Ab Initio Potentials for Helium-4 Via Second to Seventh Virial Coefficients", AIChE Annual Meeting, Orlando, FL; November 2019.
6. Apoorva Purohit, Andrew J. Schultz, Andrij Trokhymchuk and David A. Kofke, "Mapped-Averaging Formulations for Evaluation of Singlet and Multibody Density Distributions", AIChE Annual Meeting, Orlando, FL; November 2019.
7. Arpit Bansal, Akshara Goyal, Andrew J. Schultz, and David A. Kofke, "Computational cluster integral methods for solutions", AIChE Annual Meeting, Pittsburgh, PA; October 2018.
8. Navneeth Gokul, Andrew J. Schultz and David A. Kofke, "Computing Virial Coefficients to Assess the Accuracy of Intermolecular Potentials", AIChE Annual Meeting, Pittsburgh, PA; October 2018.
9. Apoorva Purohit, Sabry G. Moustafa, Arpit Bansal, Andrew J. Schultz, and David A. Kofke, "Implementation of Harmonically Mapped Averaging Methods in Popular Molecular Simulation Codebases", AIChE Annual Meeting, Pittsburgh, PA; October 2018.
10. Richard Wheatley, Andrew Schultz, Hainam Do, Navneeth Gokul and David Kofke, "Evaluation of virial coefficients and their temperature derivatives for multibody potential models", 20th Symposium on Thermophysical Properties, Boulder, CO; June 2018.
11. Weisong Lin, Sabry Moustafa, Andrew Schultz and David Kofke, "Mapped Averaging Methods for Accurate and Precise Evaluation of Free Energies and Other Properties by Molecular Simulation", 20th Symposium on Thermophysical Properties, Boulder, CO; June 2018.
12. Andrew J. Schultz, Sabry G. Moustafa, and David A. Kofke, "Mapped averages: Reformulation of statistical mechanical ensemble averages using coordinate mapping", 10th Liblice Conference on the Statistical Mechanics of Liquids, Srni (Sumava National Park), Czech Republic; June 2018.
13. Weisong Lin, Akshara Goyal, Sabry G. Moustafa, Andrew J. Schultz, David A. Kofke, "Mapped averaging methods for accurate and precise evaluation of free energies and other properties by molecular simulation", AIChE Annual Meeting, Minneapolis, MN; October 2017.
14. Navneeth Gokul, Andrew J. Schultz, David A. Kofke, Hainam Do and Richard Wheatley, "Evaluation of virial coefficients and their temperature derivatives for multibody potential models", AIChE Annual Meeting, Minneapolis, MN; October 2017.
15. Apoorva Purohit, Andrew J. Schultz, Jeffrey R. Errington and David A. Kofke, "Evaluation of defect concentrations in crystalline systems via molecular simulation", AIChE Annual Meeting, Minneapolis, MN; October 2017.
16. Andrew J. Schultz, Alexander D. Kofke, David A. Kofke, "Interactive Extensible Molecular Simulations with Etomica", AIChE Annual Meeting, Minneapolis, MN; October 2017.
17. David A. Kofke and Andrew J. Schultz, "Cluster integral methods in chemical and biological engineering", AIChE Annual Meeting, Minneapolis, MN; October 2017.
18. Sabry G. Moustafa, Andrew J. Schultz, Eva Zurek and David A. Kofke, "First-Principles Phase Diagrams: Iron at Earth's Inner Core Conditions with Full Inclusion of Anharmonic and Finite-Size Effects", AIChE Annual Meeting, San Francisco, CA; November 2016.

19. David A. Kofke, J. Ilja Siepmann, and Joan F. Brennecke, "Making Molecular Modeling and Simulation a Mainstream Source of Data for Chemical Engineering Applications", AIChE Annual Meeting, San Francisco, CA; November 2016.
20. Shu Yang, Navneeth Gokul, Andrew J. Schultz, and David A. Kofke, "Modeling of Near-Critical and Supercritical Properties Via the Virial Equation of State", AIChE Annual Meeting, San Francisco, CA; November 2016.
21. Andrew J. Schultz, Apoorva Purohit, and David A. Kofke, "Harmonically-Mapped Averaging Applied to Lennard-Jones Crystal Phase", AIChE Annual Meeting, San Francisco, CA; November 2016.
22. Andrew J. Schultz, Sabry G. Moustafa, Weisong Lin, and David A. Kofke, "High-Precision, High-Efficiency Calculation of Properties by Molecular Simulation", Fourteenth International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Porto, Portugal; May 2016.
23. Sabry G. Moustafa, Andrew J. Schultz, and David A. Kofke, "Direct calculation of anharmonic contributions to thermodynamic properties of crystals by molecular simulations", MRS Fall Meeting, Boston, MA; December 2015.
24. Andrew J. Schultz, Sabry G. Moustafa, Weisong Lin, and David A. Kofke, "Mapped averaging: Reformulation of ensemble averages for high-precision, high-efficiency calculation of properties by molecular simulation", AIChE Annual Meeting, Salt Lake City, UT; November 2015.
25. Andrew J. Schultz, Shu Yang, Ramachandran Subramanian, Allan H. Harvey, and David A. Kofke, "Molecular-based virial coefficients of pure fluids and mixtures", AIChE Annual Meeting, Salt Lake City, UT; November 2015.
26. N.S. Barlow, A.J. Schultz, S.J. Weinstein, and D.A. Kofke, "A crossover model based on the virial equation of state", Nineteenth Symposium on Thermophysical Properties, Boulder, CO; June 2015.
27. S. Moustafa, W. Lin, A.J. Schultz, and D.A. Kofke, "Crystal structure prediction of rigid-molecule crystals: Application to hydrate clathrate", AIChE Annual Meeting, Atlanta, GA; November 2014.
28. R. Subramanian, A.J. Schultz, and D.A. Kofke, "Virial coefficients of flexible molecules using path-integral Monte Carlo methods to capture nuclear quantum effects", AIChE Annual Meeting, Atlanta, GA; November 2014.
29. N.S. Barlow, A.J. Schultz, S.J. Weinstein, and D.A. Kofke, "A crossover model based on the virial equation of state", AIChE Annual Meeting, Atlanta, GA; November 2014.
30. A.J. Schultz and D.A. Kofke, "Series methods for molecularly based fluid properties prediction", 27th European Symposium on Applied Thermodynamics, Eindhoven, The Netherlands; July 2014.
31. D.A. Kofke, "Series Methods for Molecularly Based Fluid Properties Prediction", Ninth Liblice Conference on the Statistical Mechanics of Liquids, Sec Dam Lake, Czech Republic; June 2014.
32. N.S. Barlow, A.J. Schultz, D.A. Kofke, and S.J. Weinstein, "Analytical continuation of the virial series through the thermodynamic critical point", 2013 New York Conference on Applied Mathematics, Cornell University, Ithaca, NY; November 2013.
33. J.H. Yang, A.J. Schultz, J.R. Errington and D.A. Kofke, "Virial coefficient theory of adsorption of gas mixtures," AIChE Annual Meeting, San Francisco, CA; November 2013.
34. A.J. Schultz, N.S. Barlow, C. Feng, V. Chaudhary and D.A. Kofke, "Calculation of virial coefficients on graphic processors," AIChE Annual Meeting, San Francisco, CA; November 2013.

35. N.S. Barlow, A.J. Schultz, D.A. Kofke, S.J. Weinstein, "Critical Properties Extracted From Virial Series Using Approximants Consistent With Universal Scaling-Laws," AIChE Annual Meeting, San Francisco, CA; November 2013.
36. S. Yang, A.J. Schultz, D.A. Kofke, "Evaluation of Thermodynamic Properties of Gas Mixtures Via the Virial Equation of State With Accurate Molecular Models," AIChE Annual Meeting, San Francisco, CA; November 2013.
37. R. Subramanian, A.J. Schultz, D.A. Kofke, "Virial Coefficients Of Hydrogen and Nitrogen Including Quantum Effects Using Path Integral Monte Carlo", AIChE Annual Meeting, San Francisco, CA; November 2013.
38. S. Moustafa, A.J. Schultz, D.A. Kofke, "Efficient Calculation of Solid-Fluid and Solid-Solid Coexistence, Including Consideration of Point Defects", AIChE Annual Meeting, San Francisco, CA; November 2013.
39. J.H. Yang, A.J. Schultz, J.R. Errington and D.A. Kofke, "Statistical Mechanics of Fluids At Interfaces and Under Confinement Via Mayer-Sampling Monte Carlo Simulation", AIChE Annual Meeting, Pittsburgh, PA; October 2012.
40. K.R.S. Shaul, A.J. Schultz and D.A. Kofke, "An *Ab Initio* Equation of State for Supercritical Helium-4 Encapsulating Quantum Effects", AIChE Annual Meeting, Pittsburgh, PA; October 2012.
41. J.T. Golab, D.A. Kofke, and T.E. Edgar, "CACHE Update", AIChE Annual Meeting, Pittsburgh, PA; October 2012.
42. A.J. Schultz and D.A. Kofke, "Efficient Monte Carlo algorithms for simulation of crystalline solids", AIChE Annual Meeting, Pittsburgh, PA; October 2012.
43. H.M. Kim, S. Yang, A.J. Schultz, and D.A. Kofke, "Computational cluster methods for development of molecular-based equations of state: Beyond the virial equation", AIChE Annual Meeting, Pittsburgh, PA; October 2012.
44. N.S Barlow, A.J. Schultz, S.J. Weinstein, and D.A. Kofke, "An asymptotically consistent approximant method with application to soft and hard-sphere fluids", 2012 Eastern Sectional Meeting of the American Mathematical Society, Rochester, NY; September 2012.
45. C. Basaran, M. S. Sellers, A. J. Schultz, D. A. Kofke and Y. Lee, "Solder Joint Grain Boundary Structure and Self-Diffusivity via Molecular Dynamics Simulations", ITHERM 2012, San Diego, CA; May 2012.
46. T.B. Tan, A.J. Schultz, and D.A. Kofke, "Efficient, Precise and Accurate Methods of Calculating Solid-Phase Free Energies by Molecular Simulation", AIChE Annual Meeting, Minneapolis, MN; October 2011.
47. H.M. Kim, A.J. Schultz, and D.A. Kofke "Molecular Based Modeling of Polarizable Water Via Calculation of Cluster Integrals Based On Wertheim's Association Theory", AIChE Annual Meeting, Minneapolis, MN; October 2011.
48. K.R.S. Shaul, A.J. Schultz, and D.A. Kofke, "Monte Carlo Calculations of the Virial Coefficients for Development of Potential Models", AIChE Annual Meeting, Minneapolis, MN; October 2011.
49. D.A. Kofke and A.J. Schultz, "Molecular Simulation Modules for Instruction In Thermodynamics, Transport, Kinetics, and Materials", AIChE Annual Meeting, Minneapolis, MN; October 2011.
50. D.A. Kofke and T.F. Edgar, "CACHE Update", AIChE Annual Meeting, Minneapolis, MN; October 2011.
51. K.R.S. Shaul, A.J. Schultz and D.A. Kofke, "Computation of Virial Coefficients for Quantum-Mechanical Models Employing the Becke-Johnson Model of Dispersion", AIChE Annual Meeting, Salt Lake City, UT; November 2010.

52. H.M. Kim, A.J. Schultz and D.A. Kofke, "Molecular Based Modeling of Associating Fluids Via Calculation of Wertheim Cluster Integrals", AIChE Annual Meeting, Salt Lake City, UT; November 2010.
53. A.J. Schultz, K.R.S. Shaul, H.M. Kim, and D.A. Kofke, "Advances in the calculation and applications of cluster integrals for fluid property prediction", Eighth Liblice Conference on the Statistical Mechanics of Liquids, Brno, Czech Republic; June 2010.
54. M.S. Sellers, A.J. Schultz, C. Basaran, and D.A. Kofke, "Atomistic modeling of tin surface and grain boundary diffusion", AIChE Annual Meeting, Nashville, TN; November 2009.
55. K.R. Schadel, A.J. Schultz, and D.A. Kofke, "Improving the efficiency of virial-coefficient calculations: A hybrid approach employing integral-equation theories and Mayer-sampling Monte Carlo", AIChE Annual Meeting, Nashville, TN; November 2009.
56. H.M. Kim, A.J. Schultz, and D.A. Kofke, "Development of a molecular based computational approach for compressed and supercritical fluids", AIChE Annual Meeting, Nashville, TN; November 2009.
57. A.J. Schultz and D.A. Kofke, "Fluid Phase Properties using Direct Calculation of Cluster Integrals", AIChE Annual Meeting, Philadelphia, PA; November 2008.
58. D.A. Kofke, "Molecular Simulation Module Development Project Update", AIChE Annual Meeting, Salt Lake City, UT; November 2007.
59. M.S. Sellers, A.J. Schultz, D.A. Kofke, and C. Basaran, "Molecular Dynamics Modeling Of Grain Boundary Diffusion In Sn-Ag-Cu Solder", AIChE Annual Meeting, Salt Lake City, UT; November 2007.
60. D.A. Kofke, J.R. Errington and A.J. Schultz, "Progress In Developing A Web-Based Database-Driven Curriculum Assessment Tool", AIChE Annual Meeting, Salt Lake City, UT; November 2007.
61. N. Cribbin, K.M. Benjamin, A.J. Schultz, and D.A. Kofke, "Consideration of the entropy in the prediction of stable crystalline polymorphs", Eleventh International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Hersonissos, Crete, Greece; May 2007.
62. D.A. Kofke, "Assessing the accuracy of free energies calculated by molecular simulation", 233rd ACS National Meeting, Chicago, IL; March 2007.
63. K.M. Benjamin, A.J. Schultz, and D.A. Kofke, "Higher order virial coefficients and molecular clustering of polarizable water models", AIChE Annual Meeting, San Francisco, CA, November 2006.
64. N. Cribbin, A.J. Schultz, K.M. Benjamin, and D.A. Kofke, "Effective evaluation of solid-phase free energies", AIChE Annual Meeting, San Francisco, CA, November 2006.
65. A.J. Schultz, K.M. Benjamin, and D.A. Kofke, "Estimation of critical points from the virial equation of state", 2006 Midwest Thermodynamics and Statistical Mechanics Conference, Akron, OH, May 2006.
66. N. Cribbin, A.J. Schultz, K.M. Benjamin, and D.A. Kofke, "Efficient evaluation of solid-phase free energies", 2006 Midwest Thermodynamics and Statistical Mechanics Conference, Akron, OH, May 2006.
67. A.J. Schultz and D.A. Kofke, "Development and Application of Mayer Sampling Methods for the Evaluation of Cluster Integrals", AIChE Annual Meeting, Cincinnati, OH, November 2005.
68. J.K. Singh, K.M. Benjamin, and D.A. Kofke, "Cluster Integral Calculations via Mayer-Sampling Molecular Simulation: Higher-Order Virial Coefficients, Thermodynamic Properties, and Molecular Clustering", AIChE Annual Meeting, Cincinnati, OH, November 2005.

69. D. Wu and D.A. Kofke, "Improving Free Energy Calculations: Staging Sampling and Fail-Safe Bias Detection", AIChE Annual Meeting, Cincinnati, OH, November 2005.
70. S.K. Kwak and D.A. Kofke, "Strain Effects on Close-Packed Hard Sphere Crystals Containing Mono and Divacancies", AIChE Annual Meeting, Austin TX; November 2004.
71. D. Wu and D.A. Kofke, "Improving Work-based Methods for Calculating the Free Energy by Molecular Simulation", AIChE Annual Meeting, Austin TX; November 2004.
72. S.K. Kwak, J.K. Singh and D.A. Kofke, "Characterization of Thermodynamic Properties using High-order Cluster Integrals Calculated via Mayer-Sampling Molecular Simulation", AIChE Annual Meeting, Austin TX; November 2004.
73. D.A. Kofke and J.R. Errington, "Teaching Molecular Simulation using an Object Oriented Class Library", AIChE Annual Meeting, Austin TX; November 2004.
74. C.I. Iacovella, M.A. Horsch, D.A. Kofke and S.C. Glotzer, "Teaching Molecular Simulation and its Use as a Research Tool", AIChE Annual Meeting, Austin TX; November 2004.
75. J.K. Singh and D.A. Kofke, "Mayer sampling: Calculation of cluster integrals using free-energy perturbation methods", Midwest Thermodynamics and Statistical Mechanics Meeting, Buffalo, NY; June 2004.
76. Sang-Kyu Kwak and David A. Kofke, "Direct Evaluation of Coefficients of Bridge Function by Using Mayer Sampling", Midwest Thermodynamics and Statistical Mechanics Meeting, Buffalo, NY; June 2004.
77. Di Wu and David A. Kofke, "Model Study of Phase-space Overlap Measures for Free-energy Perturbation Calculations", Midwest Thermodynamics and Statistical Mechanics Meeting, Buffalo, NY; June 2004.
78. J.K. Singh and D.A. Kofke, "Effect of Molecular Association and Solutes on Vapor-liquid Interfacial Properties: A Monte Carlo Study", AIChE Annual Meeting, San Francisco, CA; November 2003.
79. D. Wu and D.A. Kofke, "Understanding Phase-space Overlap in Free Energy Calculations", AIChE Annual Meeting, San Francisco, CA; November 2003.
80. S.J. Wierzchowski and D.A. Kofke, "A Molecular Model for Hydrogen Fluoride using a New Treatment for Multibody Interactions", AIChE Annual Meeting, San Francisco, CA; November 2003.
81. J. Adhikari and D.A. Kofke, "Molecular Simulation Study of Miscibility of Compound Semiconductors", AIChE Annual Meeting, San Francisco, CA; November 2003.
82. D.A. Kofke, E.J. Maginn and R.L. Rowley, "Molecular Simulation Modules for Instruction in Thermodynamics, Transport, Kinetics and Materials", AIChE Annual Meeting, San Francisco, CA; November 2003.
83. J.K. Singh, D.A. Kofke, M. Jones and J.R. Errington, "Parallelization of Grand-canonical Ensemble Simulations for Surface Tension Calculations", AIChE Annual Meeting, San Francisco, CA; November 2003.
84. J.K. Singh and D.A. Kofke, "Effect of molecular association on interfacial properties: A Monte Carlo study", 2003 Midwest Thermodynamics and Statistical Mechanics Conference, Columbus, OH; May 2003.
85. S.K. Kwak and D.A. Kofke, "Study of vacancies in fcc hard-sphere crystals", 2003 Midwest Thermodynamics and Statistical Mechanics Conference, Columbus, OH; May 2003.
86. D. Wu and D.A. Kofke, "Understanding phase-space overlap in free energy calculations", 2003 Midwest Thermodynamics and Statistical Mechanics Conference, Columbus, OH; May 2003.
87. D.A. Kofke and S. J. Wierzchowski, "Molecular modeling study of hydrogen-fluoride/water mixtures", AIChE Annual Meeting, Indianapolis, IN; November 2002.

88. N. Lu and D.A. Kofke, "On the evaluation of potential energy differences in molecular simulation", AIChE Annual Meeting, Indianapolis, IN; November 2002.
89. D.A. Kofke and J.K. Singh, "Molecular simulation study of fundamental effects of molecular association on properties of fluid interfaces", AIChE Annual Meeting, Indianapolis, IN; November 2002.
90. D.A. Kofke and J. Adhikari, "The normal-mode Monte Carlo method for evaluation of solid-phase free energies by molecular simulation", AIChE Annual Meeting, Indianapolis, IN; November 2002.
91. N. Lu, J.K. Singh and D.A. Kofke, "Effecting Monte Carlo volume changes by localized distortions of space", AIChE Annual Meeting, Indianapolis, IN; November 2002.
92. D.A. Kofke and J. Adhikari, "Molecular simulation study of miscibility of InGaN compound semiconductors", AIChE Annual Meeting, Indianapolis, IN; November 2002.
93. S. Wierzchowski and D. A. Kofke, "Investigation of three-body forces applied to hydrogen fluoride", Midwest Thermodynamics and Statistical Mechanics Meeting, Carnegie Mellon University; May 2002.
94. J. Adhikari and D. A. Kofke, "Molecular simulation study of miscibility in InGaN compound semiconductors", Midwest Thermodynamics and Statistical Mechanics Meeting, Carnegie Mellon University; May 2002.
95. J. Adhikari and D.A. Kofke "Free energy of solids by molecular simulation", AIChE Annual Meeting, Reno, NY; November 2001.
96. D.A. Kofke "Etomica: A Java-based authoring code for teaching about and developing molecular simulations", AIChE Annual Meeting, Reno, NY; November 2001.
97. P.R. Westmoreland and D.A. Kofke "Teaching about kinetics and molecular simulations using web-based reactive molecular dynamics", AIChE Annual Meeting, Reno, NY; November 2001.
98. D.A. Kofke and S.J. Wierzchowski "Investigation of three-body forces applied to hydrogen fluoride", AIChE Annual Meeting, Reno, NY; November 2001.
99. N. Lu and D.A. Kofke "Heuristics for application of free-energy perturbation calculations in molecular simulation", AIChE Annual Meeting, Reno, NY; November 2001.
100. C.D. Barnes and D.A. Kofke, "A New Approach to Free-Energy Measurements in Solids by Molecular Simulation", AIChE Annual Meeting, Los Angeles, CA; November 2000.
101. N. Lu and D.A. Kofke, "A Very Effective Method for Completing Molecule Insertions", AIChE Annual Meeting, Los Angeles, CA; November 2000.
102. D.J. Lacks, P.T. Cummings, R.W. Rowley and D.A. Kofke, "Molecular Thermodynamics is Not an Oxymoron", AIChE Annual Meeting, Los Angeles, CA; November 2000.
103. N. Lu and D.A. Kofke, "Advances in the Understanding and Application of Molecular Simulation," Third Joint US/China Chemical Engineering Conference, Beijing, China, September 2000.
104. R. Rowley, D. Lacks, P.T. Cummings, and D.A. Kofke, "Molecular Simulation via Web-based Instruction", ASEE Annual Meeting, St. Louis, MO, June 2000 ().
105. N. Lu and D.A. Kofke, "Mistakes to avoid when computing free energies by molecular simulation", ACS Spring Meeting, San Francisco, CA, March 2000.
106. D. Visco and D.A. Kofke, "Thermodynamic Modeling of Hydrogen Fluoride", 109th Meeting of the Tennessee Academy of Science, Memphis, TN, November, 1999.
107. S. Wierzchowski, J. Gao, and D.A. Kofke, "Molecular-orbital derived empirical potential applied to hydrogen fluoride", AIChE Annual Meeting, Dallas, TX, November 1999.
108. N. Lu and D.A. Kofke, "Precision and optimization of free-energy perturbation calculations", AIChE Annual Meeting, Dallas, TX, November 1999.

109. D.A. Kofke, "Free-energy Calculations by Molecular Simulation", SUNY-Buffalo Center for Computational Research, May 1999.
110. D.A. Kofke and P.T. Cummings, "Molecular Simulations on the Web: Textbook and Modules", AIChE Annual Meeting, Miami Beach, FL, November 1998.
111. C.D. Barnes, and D.A. Kofke, "Direct Measurement of the Free Energies in Solids by Molecular Simulation", AIChE Annual Meeting, Miami Beach, FL, November 1998.
112. P. Bolhuis and D.A. Kofke, "Effect of Size Polydispersity on the Order-Disorder Transition of Hard Spheres", AIChE Annual Meeting, Miami Beach, FL, November 1998.
113. "A Study of Intermolecular Potentials for Hydrogen Fluoride", AIChE Annual Meeting, Miami Beach, FL, November 1998 (with D. Visco).
114. "Modeling Molecular Simulations", AIChE Annual Meeting, Miami Beach, FL, November 1998 (with N. Lu).
115. "A World-Wide-Web Based Textbook on Molecular Simulation", ASEE National Meeting, Seattle, WA; July 1998 (with P.T. Cummings, A.Z. Panagiotopoulos, J.J. dePablo, H.D. Cochran, D. Evans, and R. Rowley).
116. "Molecular Modeling of Hydrogen Fluoride", AIChE Annual Meeting, Los Angeles, CA; November 1997 (with D.P. Visco, Jr.).
117. "On the Computation of the Chemical Potential by Molecular Simulation", AIChE Annual Meeting, Los Angeles, CA; November 1997 (with P.T. Cummings).
118. "Modeling of Hydrogen Fluoride"; Thirteenth Symposium on Thermophysical Properties; Boulder, CO; June 1997 (with D.P. Visco, Jr. and R.R. Singh).
119. "Optimal Weighting Functions for Measuring the Chemical Potential by Molecular Simulation"; Thirteenth Symposium on Thermophysical Properties; Boulder, CO; June 1997 (with P.T. Cummings).
120. "Solid-Fluid Equilibrium in Molecular Models of n-Alkanes", AIChE Annual Meeting, Chicago, IL; November 1996.
121. "Development of a World-Wide-Web Based Textbook on Molecular Simulation", AIChE Annual Meeting, Chicago, IL; November 1996 (with P.T. Cummings).
122. "Convection-Diffusion of Solutes Through a Singular or Finite-Width Moving Interface", AIChE Annual Meeting, Chicago, IL; November 1996 (with D.S. Vaidya, J.M. Nitsche, and S.L. Diamond).
123. "Molecular Modeling of Equilibria Involving Solid Phases", CECAM Workshop on Development of Transferable Intermolecular Potentials for Phase Equilibria Calculations, Lyon, France; May 1996.
124. "Diffusion of Solutes in Polymer Liquid-Crystalline Phases: Kinetic Theory and Simulations", AIChE Annual Meeting, Miami Beach, FL; November 1995 (with A. Khare).
125. "Separations in Tunable Media", AIChE Annual Meeting, Miami Beach; November 1995 (with D. Vaidya, J. Nitsche, and S. Diamond).
126. "Molecular Simulation in Pseudo-Grand Canonical Ensembles", AIChE Annual Meeting, Miami Beach; November 1995 (with M. Mehta).
127. "Studies of Solid-Fluid Coexistence by Molecular Simulation", AIChE Annual Meeting, Miami Beach; November 1995 (with R. Agrawal).
128. "Separations in Tunable Media", 26th Annual Meeting of the Fine Particle Society, Chicago; August 1995 (with D. Vaidya, J. Nitsche, and S. Diamond)
129. "CESL: The Chemical Engineering Simulation Laboratory", Information Technology Fair, State University of New York at Buffalo; February 1995 (with M. Grosso, S. Gollapudi, N. Ingle, S. Diamond, C. Lund, T. Mountziaris, J. Nitsche, M. Ryan, and T. Weber).

130. "CESL: The Chemical Engineering Simulation Laboratory", AIChE Annual Meeting, San Francisco, CA; November 1994 (with M. Grosso, S. Gollapudi, N. Ingle, S. Diamond, C. Lund, T. Mountziaris, J. Nitsche, M. Ryan, and T. Weber).
131. "Self-diffusion in the Nematic and Smectic-A Phases of an Aligned Fluid of Hard Spherocylinders", AIChE Annual Meeting, San Francisco, CA; November 1994 (with D. Vaidya, S. Tang, and G. Evans).
132. "Efficient and Robust Evaluation of Phase Diagrams by Molecular Simulation", 12th Symposium on Thermophysical Properties, Boulder, CO; June 1994 (with R. Agrawal and M. Mehta).
133. "Phase Coexistence Properties by Molecular Simulation", Fourth Liblice Conference on the Statistical Mechanics of Liquids, Lake Milovy, Czech Republic; June 1994.
134. "Advances in the 1-1/2 Fluid Theory", AIChE Spring Meeting, Atlanta, GA; April 1994 (with H.-C. Chiu).
135. "Modeling of Inhomogeneous Systems by Hard Spheres in a Finite Periodic Narrow Box", AIChE Annual Meeting, St. Louis, MO; November 1993 (with C.J. Post).
136. "Gibbs-Duhem Integration: A New Method for Direct Evaluation of Phase Coexistence by Molecular Simulation", AIChE Spring Meeting, April, 1993 (with M. Mehta and R. Agrawal).
137. "Molecular Dynamics of Model Liquid-Crystalline Systems", AIChE Annual Meeting, Miami Beach, FL; November 1992 (with A. Khare).
138. "Monte Carlo Studies of Solute Effects in Model Nematic Systems", AIChE Annual Meeting, Los Angeles, CA; November 1991 (with R. Agrawal).
139. "Gibbs Ensemble Simulation with an Equation of State", AIChE Annual Meeting, Los Angeles, CA; November 1991 (with M. Mehta).
140. "1-1/2 Fluid Theory", Symposium on Liquids, Cornell University, Ithaca, NY; August, 1991.
141. "A Novel Approach to Conformal Solutions", AIChE Annual Meeting, Chicago, IL; November 1990.
142. "A Low-Dimensional Model for the Thermodynamics of Fluids in Narrow Pores", AIChE Annual Meeting, Chicago, IL; November 1990 (with A.J. Post).
143. "A New Conformal Solution Theory", 1990 Midwest Thermodynamics Symposium, Saw Mill Creek, OH; May 1990.
144. "Molecular Simulation Studies of Antigen-Antibody Binding", 199th National Meeting of the American Chemical Society, Boston, MA; April 1990 (with M.L. Yarmush and K.P. Antonsen).
145. "Molecular Dynamics Studies of Antigen-Antibody Interactions", AIChE Annual Meeting, San Francisco, CA; November 1989 (with M.L Yarmush and K.P. Antonsen).
146. "Infinitely Polydisperse Mixtures: A Fractal Object in Statistical Mechanics", AIChE Annual Meeting, San Francisco, CA; November 1989 (with E.D. Glandt).
147. "Computer Simulation of Phase Equilibrium", 10th IUPAC Conference on Chemical Thermodynamics, Prague, Czechoslovakia; August 1988 (with E.D. Glandt).
148. "Infinitely Polydisperse Fluids", 10th Symposium on Thermophysical Properties, Gaithersburg, MD; June 1988 (with E.D. Glandt).
149. "Monte Carlo Simulation of Multicomponent Phase Equilibria", AIChE Annual Meeting, New York, NY; November 1987 (with E.D. Glandt).
150. "Monte Carlo Simulation of Phase Equilibrium: An Application of the Semi-Grand Ensemble", AIChE Annual Meeting, Miami, FL; November 1986 (with E.D. Glandt).
151. "Monte Carlo Simulation of Continuous Mixtures", 4th International Conference on Fluid Properties and Phase Equilibria, Elsinore, Denmark; May 1986 (with E.D. Glandt).

152. "The Theory of Continuous Mixtures", AIChE Annual Meeting, Chicago, IL; November 1985 (with E.D. Glandt).
153. "Polydisperse Lennard-Jones Fluids", Royal Society of Chemistry, Multicomponent Mixtures Conference, Norwich, England; September 1985 (with E.D. Glandt).

Poster

1. Navneeth Gokul, Andrew J. Schultz, and David A. Kofke, "Virial Coefficients as a Route from Molecular Models to Accurate and Precise Thermodynamic Properties", Conference on Physical Properties and Phase Equilibria for Product and Process Design (PPEPPD), La Pineda, Spain; May 2023.
2. Sabry Moustafa, Andrew J. Schultz, and David A. Kofke, "Thermoelastic Properties of Crystals using Harmonic Mapping", Foundations of Molecular Modeling and Simulation (FOMMS), Delavan, WI; July 2022.
3. Navneeth Gokul, Andrew J. Schultz, and David A. Kofke, "Virial Coefficients as a Route from Molecular Models to Accurate and Precise Thermodynamic Properties", Foundations of Molecular Modeling and Simulation (FOMMS), Delavan, WI; July 2022.
4. Navneeth Gokul, Andrew J. Schultz, and David A. Kofke, "Virial Coefficients as a Route from Molecular Models to Accurate Thermodynamic Models", AIChE Annual Meeting (virtual), November 2020.
5. Richard A. Messerly, Navneeth Gokul, Andrew J. Schultz, David A. Kofke and Allan H. Harvey, "Molecular Calculation of the Critical Parameters of Classical Helium" AIChE Annual Meeting, Orlando, FL; November 2019.
6. Andrew J. Schultz, Christine Human, David A. Kofke, and Jeffrey R. Errington, "A Web-Based Database-Driven Assessment Management Tool", AIChE Annual Meeting, Pittsburgh PA; October 2018.
7. Apoorva Purohit, Andrew J. Schultz, Sabry G. Moustafa, Jeffrey R. Errington and David A. Kofke, "Free energy and concentration of crystalline vacancies by molecular simulation", Foundations of Molecular Modeling and Simulation (FOMMS), Delavan, WI; July 2018.
8. Sabry Moustafa, Andrew Schultz and David Kofke, "Solid-solid phase stability of metals using ab initio molecular dynamics: Application to Fe in the Earth's inner core", Foundations of Molecular Modeling and Simulation (FOMMS), Delavan, WI; July 2018.
9. Navneeth Gokul, Andrew J. Schultz, David A. Kofke, Hainam Do and Richard J. Wheatley, "Evaluation of Virial Coefficients and Their Temperature Derivatives for Multibody Potential Models", Foundations of Molecular Modeling and Simulation (FOMMS), Delavan, WI; July 2018.
10. David A. Kofke and Andrew J. Schultz, "Implementing Harmonically Mapped Averaging Methods on Popular Molecular Simulation Platforms", NSF SI2 PI Workshop, Washington, DC; May 2018.
11. Sabry G. Moustafa, Andrew J. Schultz, Eva Zurek, and David A. Kofke, "Crystal Structure at Earth's Inner Core: A First-Principles Study", American Geophysical Union (AGU) Annual Meeting, New Orleans, LA; December 2017.
12. Weisong Lin, Akshara Goyal, Andrew J. Schultz and David A. Kofke, "Mapped Averaging for Highly Efficient Evaluation of Fluid-Phase Properties By Molecular Simulation", AIChE Annual Meeting, San Francisco, CA; November 2016.

13. Nathaniel S. Barlow, Andrew J. Schultz, Steven J. Weinstein, and David A. Kofke, "Analytic Continuation of the Virial Series Through the Critical Point Using Parametric Approximants", Fourteenth International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Porto, Portugal; May 2016.
14. Andrew Schultz, Sabry Moustafa and David Kofke, "Very Efficient Methods for Evaluation of Properties of Crystalline Phases by Molecular Simulation", Foundations of Molecular Modeling and Simulation (FOMMS), Mt. Hood, OR; July 2015.
15. Weisong Lin, Andrew Schultz and David Kofke, "A Molecular-based Study of the Stability of Clathrate Hydrates", Foundations of Molecular Modeling and Simulation (FOMMS), Mt. Hood, OR; July 2015.
16. Ramachandran Subramanian, Andrew Schultz and David Kofke, "Sampling Orientations of Diatomic Molecules: Application to Path Integral Monte Carlo (PIMC) Method Including Nuclear Quantum Effects to Compute Virial Coefficients", Foundations of Molecular Modeling and Simulation (FOMMS), Mt. Hood, OR; July 2015.
17. Chao Feng, Andrew Schultz, Vipin Chaudhary and David Kofke, "Evaluation of High-order Virial Coefficients of Lennard-Jones Potential", Foundations of Molecular Modeling and Simulation (FOMMS), Mt. Hood, OR; July 2015.
18. Shu Yang, Andrew Schultz and David Kofke, "Dielectric Constants of Dilute Non-polarizable Fluids from Virial Equation of State", Foundations of Molecular Modeling and Simulation (FOMMS), Mt. Hood, OR; July 2015.
19. Nathaniel S. Barlow, Andrew J. Schultz, Steven J. Weinstein and David A. Kofke, "An Asymptotically Consistent Approximant Method with Application to Soft and Hard-Sphere fluids", AIChE Annual Meeting, Pittsburgh, PA; October 2012.
20. K.R.S. Shaul, S.G. Sankararaman, A. Schultz and D.A. Kofke, "Faster Computation of Virial Coefficients Via Mayer-Sampling Monte Carlo, Integral-Equation Theories, and Graphics Processing Units", AIChE Annual Meeting, Salt Lake City, UT; November 2010.
21. A.J. Schultz, K.R.S. Shaul, H.M. Kim, and D.A. Kofke, "Advances in the calculation and applications of cluster integrals for fluid property prediction", Twelfth International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD); May 2010.
22. T.B. Tan, N. Cribbin, A.J. Schultz, and D.A. Kofke, "Consideration of the entropy in the prediction of stable crystalline polymorphs", AIChE Annual Meeting, Nashville, TN; November 2009.
23. A.J. Schultz, T.B. Tan, N. Cribbin, and D.A. Kofke, "Analysis of free-energy methods with consideration of phase-space overlap", Foundations of Molecular Modeling and Simulation (FOMMS), Blaine, WA; July 2009.
24. A.J. Schultz, K.R. Schadel, H.M. Kim, and D.A. Kofke, "Evaluation of criticality from molecular models using the virial equation of state", Foundations of Molecular Modeling and Simulation (FOMMS), Blaine, WA; July 2009
25. T.B. Tan, N. Cribbin, A.J. Schultz, and D.A. Kofke, "Consideration Of The Entropy In The Prediction Of Stable Crystalline Polymorphs", AIChE Annual Meeting, Salt Lake City, UT; November 2007.
26. A.J. Schultz, K.M. Benjamin, and D.A. Kofke, "Calculation and analysis of virial coefficients for model systems", Eleventh International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Hersonissos, Crete, Greece; May 2007.

27. A.J. Schultz and D.A. Kofke, “Estimation of critical points from the virial equation of state”, AIChE Annual Meeting, San Francisco, CA, November 2006.
28. A.J. Schultz and D.A. Kofke, “Molecular Simulation Using a Graphical User Interface”, AIChE Annual Meeting, Cincinnati, OH, November 2005.
29. D.A. Kofke, J.K. Singh, S.-K. Kwak, and D. Wu, “Etomica: A Java-based development environment for molecular simulations”, Tenth International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Snowbird, UT; May 2004.
30. S.-K. Kwak and D.A. Kofke, “Extending the HNC integral equation theory through direct evaluation of bridge diagrams using molecular simulation”, Tenth International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Snowbird, UT; May 2004.
31. J.K. Singh and D.A. Kofke, “Molecular simulation study of surface tension of associating fluids”, Tenth International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Snowbird, UT; May 2004.
32. D. Wu and D.A. Kofke, “Understanding the influence of phase-space overlap in free energy calculations”, Tenth International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD), Snowbird, UT; May 2004.
33. D.A. Kofke, “Etomica: A Java-based API and IDE for molecular simulation”, German-American Frontiers of Engineering, Ludwigsburg, Germany; May 2003.
34. D.A. Kofke and S. J. Wierzchowski, “Computationally efficient method for treating multibody interactions in Monte Carlo simulations of associating fluids”, AIChE Annual Meeting, Indianapolis, IN; November 2002.
35. N. Lu and D. A. Kofke, “Good + bad = bad: Forward and reverse FEP calculations should not be averaged ”, Midwest Thermodynamics and Statistical Mechanics Meeting, Carnegie Mellon University; May 2002.
36. N. Lu, C.D. Barnes and D.A. Kofke, “Free-energy calculations for fluid and solid phases by molecular simulation”, Conference on Physical Properties and Phase Equilibria for Product and Process Design. Kurashiki, Japan, May 2001.
37. S. Wierzchowski and D.A. Kofke, “UB association-bias algorithm applied to the Monte Carlo simulation of hydrogen fluoride”, Conference on Physical Properties and Phase Equilibria for Product and Process Design. Kurashiki, Japan, May 2001.
38. N. Lu and D.A. Kofke, “Novel Configurational Bias Scheme for Simulation of Polymer Systems”, AIChE Annual Meeting, Los Angeles, CA; November 2000.
39. S. Wierzchowski and D.A. Kofke, “Molecular Simulation of Associating Fluids”, AIChE Annual Meeting, Los Angeles, CA; November 2000.
40. “Mistakes to avoid when computing free energies by molecular simulation,” Foundations of Molecular Modeling and Simulation (FOMMS 2000), Keystone, CO; July 2000 (with N. Lu).
41. “Molecular Simulation via Web-based Instruction,” Foundations of Molecular Modeling and Simulation (FOMMS 2000), Keystone, CO; July 2000.
42. “Molecular Modeling of Hydrogen Fluoride”, Eighth International Conference on Properties and Phase Equilibria for Product and Process Design, Noordwijkerhout, The Netherlands; May 1998 (with D. Visco).
43. “Efficient and Robust Evaluation of Phase Diagrams by Molecular Simulation”, AIChE Annual Meeting, San Francisco, CA; November 1994 (with R. Agrawal and M. Mehta).
44. “Gibbs-Duhem Integration: A New Method for Direct Evaluation of Phase Coexistence by Molecular Simulation”, Gordon Conference on the Chemistry and Physics of Liquids, Plymouth, NH, August 1993 (with R. Agrawal and M. Mehta).

45. “Molecular Dynamics Simulation of Spherical and Rodlike Solutes in a Spherocylindrical Solvent”, Gordon Conference on Liquid Crystals, Wolfeboro, NH, June 1993 (with D. Vaidya).
46. “Extensions and Applications of 1-1/2 Fluid Theory”, AIChE Annual Meeting, Miami Beach, FL; November 1992 (with H.-C. Chiu).
47. “1-1/2 Fluid Theory”, AIChE Annual Meeting, Los Angeles, CA; November 1991.
48. “A Novel Approach to Conformal Solutions”, 1991 Gordon Conference on the Chemistry and Physics of Liquids, Plymouth, NH; August 1991.
49. “Monte Carlo Studies of Freezing in Binary Hard Sphere Mixtures”, AIChE Annual Meeting, Chicago, IL; November 1990.