Andrew J. Schultz

Educational Background

Undergraduate: University of Tulsa, B.S. Chemical Engineering, 1998

Graduate: North Carolina State University, Ph.D. Chemical Engineering, 2004

Postdoctoral: State University of New York at Buffalo, Chemical and Biological Engineering, 2004-2006

Appointments

Department of Chemical and Biological Engineering, State University of New York at Buffalo

- Research Scientist (2006-2010)
- Assistant Professor of Research (2006-2020)
- Associate Professor of Research (2020-2021)

Honors and Awards

- School of Engineering and Applied Science Unsung Hero, 2020
- David Himmelblau Award for Innovations in Computer-Based Chemical Engineering Education for “the development of the etomica modules, a community-developed suite of interactive simulations to help students understand the molecular origins of macroscopic behaviors”, 2012
- Tau Beta Pi, 1997
- Phi Kappa Phi, 1998

Refereed Publications

1. N. Gokul, A. J. Schultz, D. A. Kofke, “Properties of supercritical N2, O2, CO2, andNH3 mixtures from the virial equation of state”, AIChE J. 67, e17072 (2021).
2. S. G. Moustafa, A. Purohit, A. J. Schultz, 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).
3. A. J. Schultz, D. A. Kofke, “Identifying and estimating bias in overlap-sampling free-energy calculations”, Molecular Simulation, DOI: 10.1080/08927022.2020.1758695 (2020).
4. A. Purohit, A. J. Schultz, D. A. Kofke, “Implementation of harmonically mapped averaging in LAMMPS, and effect of potential truncation on anharmonic properties”, J. Chem. Phys. 152, 014107 (2020).

5. R. J. Wheatley, A. J. Schultz, H. N. Do, N. Gokul, D. A. Kofke, “Cluster integrals and virial coefficients for realistic molecular models”, Phys. Rev. E 101, 051301 (2020).
6. R. A. Messerly, N. Gokul, A. J. Schultz, D. A. Kofke, A. H. Harvey, “Molecular Calculation of the Critical Parameters of Classical Helium”, J. Chem. Eng. Data. 65, *1028* (2020).
7. A. Trokhymchuk, A. J. Schultz, D. A. Kofke, “Alternative ensemble averages in molecular dynamics simulation of hard spheres”, Mol. Phys. 117, 3734 (2019).
8. J. R. Elliott, A. J. Schultz, D. A. Kofke, “Combined temperature and density series for fluid-phase properties. II. Lennard-Jones spheres”, J. Chem. Phys. 151, 204501 (2019).
9. A. Purohit, A. J. Schultz, D. A. Kofke, “Force-sampling methods for density distributions as instances of mapped averaging”, Mol. Phys. 117, 2822 (2019).
10. M. A. F. Afzal, A. Sonpal, M. Haghighatlari, A. J. Schultz, J. Hachmann, “A deep neural network model for packing density predictions and its application in the study of 1.5 million organic molecules”, Chem. Sci. 10, 8374-8383 (2019).
11. A. J. Schultz, D. A. Kofke, “Virial coefficients of helium-4 from ab initio based molecular models”, Journal of Chemical & Engineering Data 64, 3742 (2019).
12. K. Jain, A. J. Schultz, J. R. Errington, “Construction of the interface potential from a series of canonical ensemble simulations”, J. Chem. Phys. 151, 044103 (2019).
13. K. Jain, A. J. Schultz, J. R. Errington, “Application of the interface potential approach for studying wetting behavior within a molecular dynamics framework”, J. Chem. Phys. 150, 204118 (2019).
14. A. J. Schultz, D. A. Kofke, “Alternatives to conventional ensemble averages for thermodynamic properties”, Curr. Opin. Chem. Eng. 23, 70 (2019).
15. A. Purohit, A. J. Schultz, S. G. Moustafa, J. R. Errington, D. A. Kofke, “Free energy and concentration of crystalline vacancies by molecular simulation”, Mol. Phys. 116, 3027-3041 (2018).
16. A. Grossfield, P. N. Patrone, D. R. Roe, A. J. Schultz, D. Siderius, D. M. Zuckerman, “Best Practices for Quantification of Uncertainty and Sampling Quality in Molecular Simulations”, Living Journal of Computational Molecular Science 1, 5067 (2018).
17. A. J. Schultz, 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).
18. S. G. Moustafa, A. J. Schultz, 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).
19. W. S. Lin, A. J. Schultz, D. A. Kofke, “Electric-field mapped averaging for the dielectric constant”, Fluid Phase Equilib. 470, 17-24 (2018).

20. A. J. Schultz, S. G. Moustafa, D. A. Kofke, “No system-size anomalies in entropy of bcc iron at Earth's inner-core conditions”, Sci Rep 8, 7295 (2018).
21. S. G. Moustafa, A. J. Schultz, E. Zurek, 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).
22. M. E. Irrgang, M. Engel, A. J. Schultz, D. A. Kofke, S. C. Glotzer, “Virial Coefficients and Equations of State for Hard Polyhedron Fluids”, Langmuir 33, 11788-11796 (2017).
23. S. Yang, A. J. Schultz, D. A. Kofke, “Evaluation of second and third dielectric virial coefficients for non-polarisable molecular models”, Mol. Phys. 115, 991-1003 (2017).
24. S. G. Moustafa, A. J. Schultz, 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, 825-834 (2017).
25. R. Subramanian, A. J. Schultz, 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).
26. R. Subramanian, A. J. Schultz, D. A. Kofke, “Quantum virial coefficients of molecular nitrogen”, Mol. Phys. 115, 869-878 (2017).
27. R. Subramanian, A. J. Schultz, D. A. Kofke, “Quantum Virial Coefficients via Path Integral Monte Carlo with Semi-classical Beads”, Molecular Modeling and Simulation-Applications and Perspectives , 93-106 (2016).
28. S. Yang, A. J. Schultz, D. A. Kofke, “Thermodynamic Properties of Supercritical CO2/CH4 Mixtures from the Virial Equation of State”, J. Chem. Eng. Data 61, 4296-4312 (2016).
29. H. Do, C. Feng, A. J. Schultz, D. A. Kofke, R. J. Wheatley, “Calculation high-order virial coefficients for the square-well potential”, Phys. Rev. E 94, 013301 (2016).
30. A. J. Schultz, S. G. Moustafa, W. S. Lin, S. J. Weinstein, D. A. Kofke, “Reformulation of Ensemble Averages via Coordinate Mapping”, J. Chem. Theory Comput. 12, 1491-1498 (2016).
31. A. J. Schultz, D. A. Kofke, “Vapor-phase metastability and condensation via the virial equation of state with extrapolated coefficients”, Fluid Phase Equilib. 409, 12-18 (2016).
32. S. G. Moustafa, A. J. Schultz, D. A. Kofke, “Very fast averaging of thermal properties of crystals by molecular simulation”, Phys. Rev. E 92, 043303 (2015).
33. J. R. Elliott, A. J. Schultz, D. A. Kofke, “Combined temperature and density series for fluid-phase properties. I. Square-well spheres”, J. Chem. Phys. 143, 114110 (2015).
34. N. S. Barlow, A. J. Schultz, S. J. Weinstein, D. A. Kofke, “Communication: Analytic continuation of the virial series through the critical point using parametric approximants”, J. Chem. Phys. 143, 071103 (2015).

35. C. Feng, A. J. Schultz, V. Chaudhary, D. A. Kofke, “Eighth to sixteenth virial coefficients of the Lennard-Jones model”, J. Chem. Phys. 143, 044504 (2015).
36. A. J. Schultz, D. A. Kofke, A. H. Harvey, “Molecular-based virial coefficients of CO2-H2O mixtures”, AIChE J. 61, 3029-3037 (2015).
37. J. H. Yang, A. J. Schultz, J. R. Errington, D. A. Kofke, “The rate of convergence of the virial series in confined systems”, Mol. Phys. 113, 1179-1189 (2015).
38. S. G. Moustafa, A. J. Schultz, D. A. Kofke, “Effects of Finite Size and Proton Disorder on Lattice-Dynamics Estimates of the Free Energy of Clathrate Hydrates”, Ind. Eng. Chem. Res. 54, 4487-4496 (2015).
39. A. J. Schultz, D. A. Kofke, “Etomica: An Object-Oriented Framework for Molecular Simulation”, J. Comput. Chem. 36, 573-583 (2015).
40. A. J. Schultz, D. A. Kofke, “Quantifying Computational Effort Required for Stochastic Averages”, J. Chem. Theory Comput. 10, 5229-5234 (2014).
41. S. Yang, A. J. Schultz, D. A. Kofke, A. H. Harvey, “Interpreting Gas-Saturation Vapor-Pressure Measurements Using Virial Coefficients Derived from Molecular Models”, J. Chem. Eng. Data 59, 3183-3192 (2014).
42. N. S. Barlow, A. J. Schultz, D. A. Kofke, S. J. Weinstein “Critical isotherms from virial series using asymptotically consistent approximants”, AIChE J. 60, 3336 (2014).
43. A. J. Schultz, D. A. Kofke, “Fifth to eleventh virial coefficients of hard spheres”, Phys. Rev. E 90, 023301 (2014).
44. S. G. Moustafa, A. J. Schultz, 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).
45. H. M. Kim, A. J. Schultz, D. A. Kofke, “Second through fifth virial coefficients for model methane-ethane mixtures”, Fluid Phase Equilib. 351, 69-73 (2013).
46. J. H. Yang, A. J. Schultz, J. R. Errington, D. A. Kofke, “Calculation of inhomogeneous-fluid cluster expansions with application to the hard-sphere/hard-wall system”, J. Chem. Phys. 138, 134706 (2013).
47. A. J. Schultz, N. S. Barlow, V. Chaudhary, D. A. Kofke, “Mayer Sampling Monte Carlo calculation of virial coefficients on graphics processors”, Mol. Phys. 111, 535-543 (2013).
48. N. S. Barlow, A. J. Schultz, S. J. Weinstein, D. A. Kofke, “An asymptotically consistent approximant method with application to soft- and hard-sphere fluids”, J. Chem. Phys. 137, 204102 (2012).
49. K. R. S. Shaul, A. J. Schultz, D. A. Kofke, “Path-integral Mayer-sampling calculations of the quantum Boltzmann contribution to virial coefficients of helium-4”, J. Chem. Phys. 137, 184101 (2012).

50. K. R. S. Shaul, A. J. Schultz, D. A. Kofke, M. R. Moldover, “Semiclassical fifth virial coefficients for improved ab initio helium-4 standards”, Chem. Phys. Lett. 531, 11-17 (2012).
51. M. S. Sellers, A. J. Schultz, D. A. Kofke, C. Basaran, “Solute Effects on beta-Sn Grain Boundary Energy and Shear Stress”, J. Nanomechanics and Micromechanics 1, 41-50 (2011).
52. K. R. S. Shaul, A. J. Schultz, A. Perera, D. A. Kofke, “Integral-equation theories and Mayer-sampling Monte Carlo: a tandem approach for computing virial coefficients of simple fluids”, Mol. Phys. 109, 2395-2406 (2011).
53. K. R. S. Shaul, A. J. Schultz, D. A. Kofke, “Mayer-sampling Monte Carlo calculations of uniquely flexible contributions to virial coefficients”, J. Chem. Phys. 135, 124101 (2011).
54. A. J. Schultz, D. A. Kofke, “Algorithm for constant-pressure Monte Carlo simulation of crystalline solids”, Phys. Rev. E 84, 046712 (2011)
55. M. S. Sellers, A. J. Schultz, C. Basaran, D. A. Kofke, “Effect of Cu and Ag solute segregation on beta Sn grain boundary diffusivity”, J. Appl. Phys. 110, 013528 (2011).
56. T. B. Tan, A. J. Schultz, D. A. Kofke, “Efficient calculation of alpha- and beta-nitrogen free energies and coexistence conditions via overlap sampling with targeted perturbation”, J. Chem. Phys. 135, 044125 (2011).
57. 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. 109 123 (2011).
58. 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 55 479 (2010).
59. K.R.S. Shaul, A.J. Schultz, and D.A. Kofke, “Mayer-sampling Monte Carlo calculations of methanol virial coefficients”, Molec. Sim. 36 1282 (2010).
60. 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 134104 (2010).
61. A.J. Schultz and D.A. Kofke, "Virial coefficients of model alkanes", J. Chem. Phys. 133 104101 (2010).
62. H.M. Kim, A.J. Schultz, D.A. Kofke, "Molecular based modeling of associating fluids via calculation of Wertheim cluster integrals", J. Phys. Chem. B 114 11515 (2010).
63. 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).
64. M.S. 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).

65. 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].
66. 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).
67. 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).
68. A.J. Schultz and D.A. Kofke, “Sixth, seventh and eighth virial coefficients of the Lennard-Jones model”, Mol. Phys. 107 2309-2318 (2009).
69. A.J. Schultz and D.A. Kofke, “Virial coefficients of Lennard-Jones mixtures”, J. Chem. Phys. 130 224104/1-9 (2009).
70. A.J. Schultz and D.A. Kofke, “Interpolation of virial coefficients”, Molec. Phys. 107(14), 1431-1436 (2009).
71. 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).
72. S. Li, M.S. Sellers, C. Basaran, A.J. Schultz, and D.A. Kofke, “Lattice Strain Due to an Atomic Vacancy", Int. J. Mol. Sci. 10 2798 (2009).
73. K.M. Benjamin, A.J. Schultz and D.A. Kofke, “Fourth and Fifth Virial Coefficients of Polarizable Water”, J. Phys. Chem. B 111 16021-16027 (2009).
74. K.M. 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 16021-16027 (2007).
75. K.M. Benjamin, A.J. Schultz, J. K. Singh and D.A. Kofke, “Higher-order virial coefficients of water models”, J. Phys. Chem. B 111 11463-11473 (2007).
76. A.J. Schultz, C.K. Hall and J. Genzer, “Obtaining concentration profiles from computer simulation structure factors”, Macromolecules 40 2629-2632 (2007).
77. K.M. Benjamin, A.J. Schultz and D.A. Kofke, “Gas-Phase molecular clustering of TIP4P and SCP/E water models from higher-order virial coefficients”, Ind. Eng. Chem. Res. 45 5566-5573 (2006).
78. A.J. Schultz, C.K. Hall and J. Genzer, “Computer Simulation of Block Copolymer/Nanoparticle Composites”, Macromolecules 38 3007-3016 (2005).
79. A.J. Schultz, C.K. Hall and J. Genzer, “Box Length Search Algorithm for Molecular Simulation of Systems Containing Periodic Structures”, J. Chem. Phys. 120 2049 (2004).
80. A.J. Schultz, C.K. Hall and J. Genzer, “Computer Simulation of Copolymer Phase Behavior”, J. Chem. Phys. 117 10329-10338 (2002).

Teaching Experience

Co-taught Molecular Modeling, University at Buffalo, Fall 2007.

- Responsibility for teaching classes related to use of Etomica molecular simulation software.
- Helped students design simulations

Graduate students in the Kofke group, 2006-present.

- Supervision of students during development and analysis of molecular simulations
- Co-authorship of 46 refereed journal articles with 12 students and 2 post-docs.

Service to the University

- Website maintainer (2006-2020) and web application developer for the Department of Chemical and Biological Engineering since 2006.
- Web application developer for the School of Engineering and Applied Sciences Office of Undergraduate Education since 2015.

Research Support

- National Science Foundation, CHE-CTMC: Development of Molecular Simulation Methods to Compute Phase and Interfacial Properties of Complex Fluids, 6/1/2019-5/31/2022
- National Science Foundation, SI2-SSE: Infrastructure Enabling Broad Adoption of New Methods That Yield Orders-of-Magnitude Speedup of Molecular Simulation Averaging, 10/01/2017 - 9/30/2021
- National Science Foundation (CHE), CDS&E: Development and application of cluster-integral methods for dispersions and complex solutions, 6/15/2015-5/31/2020
- National Science Foundation (CBET), UNS: Detailed molecular-thermodynamics methods for high-precision calculation of condensation, criticality and supercritical behaviors of fluids and fluid mixtures, 6/15/2015 - 5/31/2021
- Petroleum Research Fund of the ACS, “A Comprehensive Molecular-Based Study of the Stability of Clathrate Hydrates”, 6/1/2013 - 8/31/2015
- National Science Foundation, “New cyber-enabled strategies to realize the promise of quantum chemistry as a far-reaching tool for engineering applications”, 10/1/2010 - 9/30/2015
- National Science Foundation, “Modeling of fluids and interfaces via synthesis of integral equations and Mayer-sampling cluster integral calculations”, 9/1/2009 - 8/31/2012

Professional Society Membership

- American Institute of Chemical Engineers, Senior Member

Invited Presentations

1. S. G. Moustafa, A. J. Schultz, D. A. Kofke, “Very Efficient Methods for Evaluation of Properties of Crystalline Phases by Molecular Simulation”, Nineteenth Symposium on Thermophysical Properties, Boulder, CO; 2015.

Contributed Presentations (underline indicates speaker)

1. David A. Kofke, Sabry G. Moustafa, Andrew J. Schultz, Francis W. Starr and Jack F. Douglas, “Quantifying Dynamic Heterogeneity of Glasses: Percolation Perspective”, AIChE Annual Meeting, Orlando, FL; November 2019.
2. Yiqi Chen, Andrew J. Schultz, Jeffrey R. Errington, “Molecular Simulation on the Antifouling Mechanism of Zwitterionic Materials”, AIChE Annual Meeting, Orlando, FL; November 2019.
3. 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.
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. Karnesh Jain, Andrew J. Schultz and Jeffrey R. Errington, “Development of Interface Potential Based Methods for Calculating the Wetting Properties of Complex Systems”, AIChE Annual Meeting, Pittsburgh, PA; October 2018.
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. 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.
32. 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.
33. 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.
34. 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.
35. 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.
36. 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.
37. 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.
38. 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.
39. 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.

40. A.J. Schultz and D.A. Kofke, “Efficient Monte Carlo algorithms for simulation of crystalline solids”, AIChE Annual Meeting, Pittsburgh, PA; October 2012.
41. 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.
42. 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.
43. 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.
44. 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.
45. 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.
46. 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.
47. 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.
48. 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.
49. 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.
50. 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.
51. 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.
52. 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.
53. 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.
54. A.J. Schultz and D.A. Kofke, “Fluid Phase Properties using Direct Calculation of Cluster Integrals”, AIChE Annual Meeting, Philadelphia, PA; November 2008.

55. D.A. Kofke, “Molecular Simulation Module Development Project Update”, AIChE Annual Meeting, Salt Lake City, UT; November 2007.
56. 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.
57. 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.
58. 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.
59. 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.
60. 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.
61. 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.
62. 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.
63. 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.
64. Andrew J. Schultz, Carol K. Hall, Jan Genzer, “Computer Simulation of Block Copolymer Copolymer Phase Behavior”, 2002 American Physical Society Annual Meeting, Indianapolis, IN, March 2002.

Posters

1. 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.
2. 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.
3. 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.
4. 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.

5. 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.
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. 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.
8. 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.
9. 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.
10. 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.
11. 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.
12. 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.
13. 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.
14. 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.
15. 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.
16. 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.
17. 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.
18. 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.

19. 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.
20. 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.
21. 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
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, Salt Lake City, UT; November 2007.
23. 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.
24. 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.
25. A.J. Schultz and D.A. Kofke, “Molecular Simulation Using a Graphical User Interface”, AIChE Annual Meeting, Cincinnati, OH, November 2005.
26. Andrew Schultz, Carol Hall, Jan Genzer, “Computer Simulation of Copolymer Phase Behavior”, 2001 American Physical Society Annual Meeting, Seattle, WA, March 2001.

Workshops Conducted

1. D. A. Kofke and A. J. Schultz, “Uncertainty estimation in molecular simulation”, FOMMS 2018, Lake Lawn Resort, Delevan, WI; July 2018.
2. D. A. Kofke and A. J. Schultz, “Using interactive molecular simulations to help students understand thermo, transport, and kinetics”, ASEE Summer School 2017, North Carolina State University; July 2017.
3. D. A. Kofke and A. J. Schultz, “Open-source molecular simulation standards”, FOMMS 2009, Semiahmoo Resort, Blaine, WA; July 2009.
4. D. A. Kofke and A. J. Schultz, “Molecular simulation modules”, FOMMS 2009, Semiahmoo Resort, Blaine, WA; July 2009.