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Education

Ph.D. Chemistry, University of California, Santa Cruz, *2018*.

- Thesis title: "Theoretical Studies of Molecular Structure, Dynamics, and Reactivity at Liquid Interfaces."
- Chancellor's Dissertation-Year Fellowship, 2017
- American Chemical Society's Chemical Computing Group Excellence Award for Graduate Students, 2017

M.S. Chemistry, University of California, Irvine, *2006*.

- Graduate Assistance in Areas of National Need (GAANN) Fellowship, 2004

B.S. Chemical Engineering, University of Kentucky, *1999*.

- University of Kentucky National Merit Scholarship, 1994
- Dean James Hiram Graham Memorial Scholarship, 1997

Publications

21. Barnett, A. Karnes, J. J.; Major, D. R.; Oakdale, J. S.; Grew, K. N.; McClure, J. P.; Molinero, V. Exponential Water Uptake in Ionomer Membranes Results from Polymer Plasticization. *Macromolecules* **2022**, *55*, 6762–6774.

20. Karnes, J. J.*; Weisgraber, T. H.; Cook, C. C.; Fox, C. A.; Harris, B. S.; Oakdale, J. S.; Faller, R. Shusteff, M. Isolating the Reaction Mechanism as a Variable with Coarse-Grained Reactive Molecular Dynamics: Step-Growth versus Chain-Growth Polymerization. (*arXiv:2210.01758*)

19. Karnes, J. J.*; Weitzner, S. E.; Akhade, S. A.; Baker, S. A.; Duoss; E. B.; Varley, J. B. A Hybrid Quantum-Classical Study of Ion Adsorption at the Copper Electrode. *J. Phys. Chem. C* **2022**, *126*, 12413-12423.

18. Ramesh, V.; Giera, B.; Karnes, J. J.; Stratman, N.; Schaufler, V.; Li, Y.; Rehbock, C.; Barcikowski, S. Electrophoretic Deposition of Platinum Nanoparticles using Ethanol-Water Mixtures Significantly Reduces Neural Electrode Impedance. *J. Electrochem. Soc.* **2022**, *169*, 022504

17. Ramesh, V.; Rehbock, C.; Giera, B.; Karnes, J. J.; Angelov, S. D.; Schwabe, K.; Barcikowski, S. Comparing Direct and Pulsed-Direct Current Electrophoretic Deposition on Neural Electrodes: Deposition Mechanism and Functional Influence. *Langmuir* **2021**, *37*, 9724–9734.

16. Karnes, J. J.*; Benjamin, I. Deconstructing the Local Intermolecular Ordering and Dynamics of Liquid Chloroform and Bromoform. *J. Phys. Chem. B* **2021**, *125*, 3629–3637.

15. Melchert, D. S.; Johnson, K.; Giera, B.; Fong, E. J.; Shusteff, M.; Mancini, J.; Karnes, J. J.; Cobb, C. L.; Spadaccini, C.; Gianola, D. S.; Begley, M. R. Modeling Meso- and Microstructure in Materials Patterned with Acoustic Focusing. *Mater. Des.* **2021**, *202*, 109512.

14. Karnes, J. J.*; Weisgraber, T. H.; Oakdale, J. S.; Mettry, M.; Shusteff, M; and Biener, J. On the Network Topology of Crosslinked Acrylate Photopolymers: A Molecular Dynamics Case Study. *J. Phys. Chem. B* **2020**, *124*, 9204-9215. *Supplementary cover image.*

13. Karnes, J. J.; Villavicencio, N.; Benjamin, I. Transfer of an Erbium Ion across the Water/Dodecane Interface: Structure and Thermodynamics via Molecular Dynamics Simulations. *Chem. Phys. Lett.* **2019**, *737*, 136825.

12. Karnes, J. J.; Benjamin, I. Miscibility at the Immiscible Liquid/Liquid Interface: A Molecular Dynamics Study of Thermodynamics and Mechanism. *J. Chem. Phys.* **2018**, *148*, 034707.

11. Karnes, J. J.; Benjamin, I. On the Local Intermolecular Ordering and Dynamics of Liquid Chloroform. *J. Mol. Liq.* **2017**, *248*, 121-126.

10. Karnes, J. J.; Benjamin, I. S_N2 Reaction Rate Enhancement by β-cyclodextrin at the Liquid/Liquid Interface. *J. Phys. Chem. C* **2017**, *121*, 19209-19217.

9. Karnes, J. J.; Benjamin, I. Structure and Dynamics of Host/Guest Inclusion Complexes at the Liquid/Liquid Interface: Implications for Inverse Phase Transfer Catalysis. *J. Phys. Chem. C* **2017**, *121*, 4999-5011.

8. Karnes, J. J.; Benjamin, I. Geometric and Energetic Considerations of Surface Fluctuations During Ion Transfer Across the Water-Immiscible Organic Liquid Interface. *J. Chem. Phys.* **2016**, *145*, 014701. *Journal cover image.*

7. Karnes, J. J.; Gobrogge, E. A.; Walker, R. A.; Benjamin, I. Unusual Structure and Dynamics at Silica/Methanol and Silica/Ethanol Interfaces: A Molecular Dynamics and Nonlinear Optical Study. *J. Phys. Chem. B* **2016**, *120*, 1569-1578.

6. Karnes, J. J.; Benjamin, I. Mechanism and Dynamics of Molecular Exchange at the Silica/Binary Solvent Mixtures Interface. *J. Phys. Chem. A* **2015**, *119*, 12073-12081.

5. Sethian, J. D.; *et. al.* The Science and Technologies for Fusion Energy with Lasers and Direct-Drive Targets. *IEEE Trans. Plasma Sci.* **2010**, *38*, 690-703.

4. Karnes, J. J.*; Petta, N. M.; Streit, J. E. Optimization of Phase Transfer Catalysis for in Situ Coating of Resorcinol Formaldehyde Targets. *Fusion Sci. Technol.* **2009**, *55*, 472-476.

3. Rearden, P.; Harrington, P. B.; Karnes, J. J.; Bunker, C. E. Fuzzy Rule-Building Expert System Classification of Fuel Using Solid-Phase Microextraction Two-Way Gas Chromatography Differential Mobility Spectrometric Data. *Anal. Chem.* **2007**, *79*, 1485-1491.

2. Wang, G.; Karnes, J. J.; Bunker, C. E.; Lei Geng, M. Two-Dimensional Correlation Coefficient Mapping in Gas Chromatography: Jet Fuel Classification for Environmental Analysis. *J. Mol. Struct.* **2006**, *799*, 247-252.

1. Bunker, C. E.; Karnes, J. J. Low-Temperature Stability and High-Temperature Reactivity of Iron-Based Core-Shell Nanoparticles. *J. Am. Chem. Soc.* **2004**, *126*, 10852-10853.

* *as corresponding author*

Presentations

26. Karnes, J. J.; Weisgraber, T. H.; Fox, C. A.; Harris, B. S.; Cook, C. C.; Wang, D. N.; Oakdale, J. S.; Faller, R.; Shusteff, M. "Photopolymer Resin Design with Reactive Coarse-Grained Molecular Dynamics: Reaction Mechanism as a Variable" Oral, Materials Research Society, Fall 2021, Boston, MA, 1 December 2021.

25. Karnes, J. J.; Weisgraber, T. H.; Harris, B. S.; Fox, C. A.; Oakdale, J. S.; Faller, R.; Shusteff, M. "Isolating the Reaction mechanism as a variable: Reactive coarse-grained molecular dynamics simulation of chain-growth versus step-growth polymerization." Oral, American Chemical Society, Spring 2021, virtual, 14 April 2021.

24. Karnes, J. J.; Weisgraber, T. H.; Oakdale, J. S.; Shusteff, M; Biener, J. "Network topology of crosslinked acrylate polymers." Poster, Berkeley Statistical Mechanics Meeting, University of California, Berkeley, CA, 11 January 2020.

23. Karnes, J. J.; Weisgraber, T. H.; Oakdale, J. S.; Shusteff, M.; Biener, J. "Toward photopolymer resin design for additive manufacturing." Poster, 6th LAMMPS Workshop and Symposium, Albuquerque, NM, 15 August 2019.

22. Karnes, J. J.; Weisgraber, T. H.; Oakdale, J. S.; Biener, J. "An Atomistic Approach toward Modelling Additive Manufacturing." Oral, 257th American Chemical Society National Meeting & Exposition, 31 March 2019.

21. Karnes, J. J.; Weisgraber, T. H.; Biener, J.; Oakdale, J. S.; Shusteff, M. "An Atomistic Approach toward Modelling Additive Manufacturing." Poster, Berkeley Statistical Mechanics Meeting, University of California, Berkeley, CA, January 2019.

20. Karnes, J. J.; Benjamin, I. "Mixing oil and water: The thermodynamics and mechanism of water transferring into oil." Poster, West Coast Theoretical Chemistry Symposium, Stanford University, 28 March 2018.

19. Karnes, J. J.; Benjamin, I. "Influence of Surface-Active Molecules on Reactions at Liquid Interfaces: Molecular Dynamics Studies." Oral, 255th American Chemical Society National Meeting & Exposition, New Orleans, LA, 18 March 2018.

19. Karnes, J. J.; Benjamin, I. "Mixing oil and water: The thermodynamics and mechanism of water transferring into oil." Poster, 255th American Chemical Society National Meeting & Exposition, New Orleans, LA, 20 March 2018.

18. Karnes, J. J.; Benjamin, I. "Mixing oil and water: The thermodynamics and mechanism of water transferring into oil." Poster, University of California, Santa Cruz Postdoc Symposium, Santa Cruz, CA, 1 March 2018.

17. Karnes, J. J.; Benjamin, I. "Mixing oil and water: The thermodynamics and mechanism of water transferring into oil." Poster, Berkeley Statistical Mechanics Meeting, University of California, Berkeley, CA, 12 January 2018.

16. Karnes, J. J.; Benjamin, I. "Deconstructing inverse phase transfer catalysis with computer simulations." Oral, University of California, Santa Cruz Department of Chemistry and Biochemistry Conference, Santa Cruz, CA, 19 September 2017.

15. Karnes, J. J.; Benjamin, I. "Quantifying the catalyst's role in inverse phase transfer catalysis with computer simulations." Oral, 253rd American Chemical Society National Meeting & Exposition, San Francisco, CA, 4 April 2017.

14. Karnes, J. J.; Benjamin, I. "Water Transfer at the Water/Oil Interface." Oral, 2nd University of California Chemical Symposium, Lake Arrowhead, CA, 28 March 2017.

13. Karnes, J. J.; Benjamin, I. "Local Ordering in Chloroform and Carbon Tetrachloride." Poster, University of California, Berkeley Mini Statistical Mechanics Meeting, 14 January 2017.

12. Karnes, J. J.; Benjamin, I. "Simulating a Host/Guest System at the Liquid/Liquid Interface." Poster, University of California, Santa Cruz Department of Chemistry and Biochemistry Conference, 13 September 2016.

11. Karnes, J. J.; Benjamin, I. "Deconstructing the 'water finger': A re-examination of water-organic ion transfer." Poster, University of California Symposium for the Chemical Sciences, Lake Arrowhead, CA, 22 March 2016.

10. Karnes, J. J.; Benjamin, I. "Deconstructing the 'water finger': A re-examination of water-organic ion transfer." Poster, 251st American Chemical Society National Meeting & Exposition, San Diego, California, 14-16 March 2016.

9. Karnes, J. J.; Benjamin, I. "Ion transfer across a water-nitrobenzene interface." Poster, University of California, Santa Cruz Department of Chemistry and Biochemistry Conference, 9 September 2015.

8. Karnes, J. J.; Benjamin, I. "Investigating a Binary Solvent Mixture at the Liquid-Solid Interface via Molecular Dynamics." Oral, Tohoku University Chemistry Summer School, Sendai, Japan, 27 August 2015.

7. Karnes, J. J.; Benjamin, I. "Binary solvents at liquid-solid interfaces: hydrogen bond competition." Poster, University of California, Santa Cruz Department of Chemistry and Biochemistry Conference, 16 September 2014.

6. Karnes, J. J.; *et. al.* "Progress toward an air-dried HAPL target capsule" 51st Annual Meeting of the American Physical Society Division of Plasma Physics, Atlanta, GA, 2-6 November 2009.

5. Karnes, J. J.; *et. al.* "Progress on Air Dried RF foam shells and In-situ Coatings" 19th High Average Power Laser Program Workshop, University of Wisconsin, Madison, 22-23 October 2008.

4. Karnes, J. J. *et. al.* "In Situ Resorcinol Formaldehyde Coatings" 18th Target Fabrication Meeting, Lake Tahoe, CA, 11-15 May 2008.

3. Karnes, J. J.; *et. al.* "In Situ Resorcinol Formaldehyde Coatings" 17th High Average Power Laser Program Workshop, Naval Research Laboratory, Washington, DC, 30-31 October 2007.

2. Karnes, J. J; Sanders, N. L.; Guliants, E. A.; Bunker, C. E. "Preparation, Characterization, and Reactivity of Iron Core-Shell Nanoparticles," 2nd Annual Nano-Materials for Defense Applications Symposium, Maui, HI, February 2004.

1. Karnes, J. J.; *et. al.* "Predicting the Physical Properties of Aviation Fuels through Advanced Chemometric Analysis of Analytical Data" 28th Dayton-Cincinnati Aerospace Sciences Symposium, Dayton, OH, 4 March 2003.

Service and Outreach

ad hoc reviews for *Nature Communications, The Journal of Physical Chemistry, Scientific Reports, Materials Communications, Journal of Molecular Liquids, Chemistry Communications, etc.*

Lawrence Livermore National Laboratory's "STEM Day" Volunteer, 2018 & 2019.

"Dine with a Scientist," 2019 & 2020, Irvington High School, Fremont, CA.

Committee member for the 2017 and 2018 University of California Chemical Symposiums. Serving on the Grant Writing, Fundraising, and Oral & Poster Session Planning subcommittees. *Secured NSF grant 1707956, February 2017. Secured Army Research Office grant W911NF-18-1-0039, November 2017.*

Volunteer as an "expert" with *Science Buddies*, a nonprofit organization that helps students, parents, and teachers with the design and implementation of K-12 science fair experiments.

Presented lecture, "Update from a Boyd County Middle School Graduate" to middle school 'Careers in STEM' class, 2 November 2022.

Teaching Experience

Teaching Assistantships: General Chemistry Lecture, General Chemistry Laboratory, Scientific Computing Skills (with Mathcad)

Substitute Lecturer: General Chemistry

Previous Positions

Schafer Corporation, *Senior Scientist*, Livermore, CA. *2006-2011.*

Innovative Scientific Solutions, Inc., *Research Engineer*, Wright Patterson Air Force Base, Dayton, OH. *2002-2004.*

AK Steel, *Maintenance Area Manager*, Middletown, OH. *1996-2002.*

Additional information and training

Currently hold U.S. Department of Energy 'Q' security clearance. Previously held U.S. Department of Defense 'Top Secret' security clearance.

"Stanford/PULSE Electronic Structure Summer School," short course, Stanford/SLAC National Accelerator Laboratory, Menlo Park, CA, June 2017.

"Nuclear Forensic Science," short course, Radiochemistry Society, Richland, WA, January 2011.

"Environmental Radiochemistry," short course, Nevada Technical Associates, Inc., Roswell, GA, April 2010.

"Polymer Chemistry: Principles and Practice," short course, American Chemical Society, Blacksburg, VA, April 2007.

"ISO 9001:2000 - Fundamentals," short course, QMI Management Systems Registration, Edmonton, AB, June 2006.

Selected programming languages and computer environments

LAMMPS (open source project, molecular dynamics engine of choice) Recent customizations: `fix sticky`, `fix infect`, and `fix cure`

VMD (preferred MD visualization)

Quantum ESPRESSO (plane-wave DFT, familiarity with DFT/ESM-RISM)

gnuplot (publication-ready spatial distribution function plots)

C (primary programming language, go-to for data analysis and handling), C++ (LAMMPS customization)

Python (data analysis, NetworkX, etc.)

High-performance computing, Slurm and LSF job scheduling

Linux environments, shell scripting, sed/awk, etc.

C# (instrument control, GUI)

MATLAB (general usage, chemometric data analysis: partial least squares, principal component analysis, etc.)

LaTeX(doctoral thesis, journal articles)