

James “Wes” Barnett

Molecular Modeler · Chemical Engineer

Curriculum Vitae · March 2018

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I am a postdoctoral research scientist in Chemical Engineering. My current research focuses on using computer simulations to study nanocomposite membranes. My interests include polymer physics, statistical thermodynamics, molecular simulation, multi-scale modeling of self-assembly, and solution thermodynamics.

SKILLS

- **Simulation packages:** LAMMPS, GROMACS, AmberTools, Gaussian
- **Data analysis:** scikit-learn, Keras, R
- **Programming:** Modern Fortran, C++, Python, bash, git
- **Visualization:** L^AT_EX, vmd, gnuplot, GIMP, ImageMagick
- **Simulation and analysis techniques:** free energy simulations, replica exchange, window sampling, machine learning

EDUCATION

2017	Ph.D., Chemical and Biomolecular Engineering Tulane University, New Orleans, LA	GPA 3.94/4.00
2011	M.Div. New Orleans Baptist Theological Seminary, New Orleans, LA	GPA 4.00/4.00
2007	B.S., Mechanical Engineering Mississippi State University, Starkville, MS	GPA 3.78/4.00

PROFESSIONAL & RESEARCH EXPERIENCE

2017–	Postdoctoral Research Scientist <i>Columbia University, New York City, NY</i> PI: Sanat Kumar. Plan, setup, perform, and analyze molecular simulations of polymer and nanocomposite systems. Investigate nanoparticle miscibility and gas separation processes. Develop theory regarding these processes and systems.
2012–17	Research Assistant <i>Tulane University, New Orleans, LA</i> PI: Hank Ashbaugh. Plan, setup, perform, and analyze molecular simulations investigating guest-host interactions, packing effects, dewetting, and the hydrophobic effect.

- 2010–12 **Engineer-In-Training**
Schultz and Summers Engineering, Kenner, LA.
Tested soil, concrete, aggregate, and asphalt. Performed equipment calibrations and trained employees. Reported results to contractors.
- 2003–05 **Engineering Co-op**
Grand Gulf Nuclear Station, Port Gibson, MS
Co-op job in conjunction with Mississippi State University, alternating semesters, totaling 14 months. Engineering Programs. Collected vibration readings and infrared thermography data on plant equipment and assisted engineers in analysis. Corrected fire pre-plans and revised plant procedures.

PUBLICATIONS

1. Tang, D.; **Barnett, J. W.**; Tang, D.; Gibb B. C.; Ashbaugh, H. S. Alkane guest packing drives switching between multimeric deep-cavity cavitated assembly states *Chem. Comm.* **2018**. DOI: 10.1039/C8CC00036K.
2. Tang, D.; **Barnett, J. W.**; Gibb B. C.; Ashbaugh, H. S. Guest controlled non-monotonic deep cavity cavitated assembly state switching. *J. Phys. Chem. B.* **2017**, *121* 10717–10725. DOI: 10.1021/acs.jpcc.7b09021.
3. Ashbaugh, H. S.; **Barnett, J. W.**; Saltzman A.; Langrehr, M.; Houser, H. Connections between the anomalous volumetric properties of alcohols in aqueous solution and the volume of hydrophobic association. *J. Phys. Chem. B.* **2017**. DOI: 10.1021/acs.jpcc.7b08728.
4. **Barnett, J. W.**; Bhutta, A.; Briebier, S. C.; da Silva Moura, N.; Ashbaugh, H. S. Resolving solvophobic interactions inferred from experimental solvation free energies and evaluated from molecular simulation. *Chem. Phys. Lett.* **2017**, *667*, 62–67. DOI: 10.1016/j.cplett.2016.11.038.
5. Ashbaugh, H. S.; **Barnett, J. W.**; Saltmann, A.; Langrehr, M.; Houser, H. Stiffening of dilute alcohol and alkane mixtures with water *J. Chem. Phys.* **2016**, *145*, 201102, DOI:10.1063/1.4971205.
6. **Barnett, J. W.**; Gibb, B. C.; Ashbaugh, H. S. Succession of alkane conformational motifs bound within hydrophobic supramolecular capsular assemblies. *J. Phys. Chem. B.* **2016**, *120* (39), 10394–10402, DOI: 10.1021/acs.jpcc.6b06496.
7. Ashbaugh, H. S.; da Silva Moura, N.; House, H.; Wang, Y.; Goodson, A.; **Barnett, J. W.** Temperature and pressure dependence of the interfacial free energy against a hard surface in contact with water and decane. *J. Chem. Phys.* **2016**, *145*, 124710, DOI: 10.1063/1.4963692.
8. Ashbaugh, H. S.; **Barnett, J. W.**; da Silva Moura N.; Houser, H. E. Hydrated nonpolar solute volumes: Relationships between size, attractiveness, and molecular structure. *Biophysical Chemistry.* **2016**, *213*, 1–5, DOI: 10.1016/j.bpc.2016.03.002.

CONFERENCE PRESENTATIONS

Only presentations where I was the presenting author are listed.

1. Coarse-grained simulations of gas penetrants in polymer nanocomposites. APS March Meeting. Mar 5–9, 2018.
2. Assembly-state switching: Alkane guest length drives assembly transitions between multimeric deep-cavity cavitand complexes. AIChE Annual Meeting. Nov 13–18, 2016.
3. Resolving experimentally-inferred solvophobic interactions in the overlap region. Poster. AIChE Annual Meeting. Nov 13–18, 2016.
4. Progression of conformational transitions of alkanes under hydrophobic confinement in deep-cavity cavitand dimer complexes. AIChE Annual Meeting. Nov 8–13, 2015.
5. A molecular dynamics study of the confinement of alkane guests in an octa-acid dimer. Poster. ACS National Meeting. Mar 22–26, 2015.

FELLOWSHIPS, SCHOLARSHIPS, & AWARDS

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| 2016 | Outstanding Scholarship Award, Tulane Department of Chemical and Biomolecular Engineering |
| 2016 | Outstanding Research Award, Tulane Department of Chemical and Biomolecular Engineering |
| 2016 | Tulane GSSA/OGPS Travel Award, AIChE Annual Meeting. |
| 2016 | Tulane School of Science & Engineering Travel Award, AIChE Annual Meeting. |
| 2015 | Tulane GSSA/OGPS Travel Award, AIChE Annual Meeting. |
| 2015 | Tulane School of Science & Engineering Travel Award, AIChE Annual Meeting. |
| 2015 | Tulane GSSA/OGPS Travel Award, ACS National Meeting. |
| 2015 | Tulane School of Science & Engineering Travel Award, ACS National Meeting. |
| 2013–17 | Louisiana Board of Regents Graduate Fellowship, Tulane University. |
| 2003 | Outstanding Honors Freshman, Mississippi State University. |
| 2002–07 | Mississippi Eminent Scholars Grant, Mississippi State University. |
| 2002–07 | Hunter Henry Scholarship, Mississippi State University. |

TEACHING EXPERIENCE

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| 2017 | Attended workshop on Evidence-based Teaching in STEM, Columbia University. |
| 2014–17 | Research Mentor. Consistently mentored and supervised 2-3 undergraduate students, Tulane University. |
| 2013 | Teaching Assistant. Thermodynamics, Tulane University. |
| 2012 | Teaching Assistant. Material and Energy Balances, Tulane University. |

UNIVERSITY SERVICE & COMMUNITY OUTREACH

- 2016 Science fair judge. Chateau Estates Elementary School, Kenner, LA.
- 2015 Mentor to international student. Tulane University Office of International Students and Scholars.
- 2014–15 Science fair pre-review volunteer. Greater New Orleans Science and Engineering Fair, New Orleans, LA.
- 2013–17 Tulane Graduate Honor Board, Officer.
- 2013–14 Tulane Chemical & Biomolecular Engineering Graduate Student Association, President.
- 2012–14 International student events coordinator. Tulane Baptist Collegiate Ministry.

PROFESSIONAL MEMBERSHIPS

American Institute of Chemical Engineers
American Physical Society