DR. DAVID S. SIMMONS

Assistant Professor of Polymer Engineering

Glass Formation, Polymer Theory, Molecular Simulation

THE UNIVERSITY OF AKRON

Department of Polymer Engineering
The University of Akron, OH
330-972-6675
dsimmon@uakron.edu
blogs.uakron.edu/simmonsgroup/

Biography: David Simmons, an expert in computational materials design, soft matter physics, and polymer physics, joined UA in 2012 from the National Institute of Standards and Technology (NIST) in Gaithersburg MD., where he completed a postdoctoral fellowship focused on simulation of polymer glass formation. Simmons received his Ph.D. in Chemical Engineering at the University of Texas, Austin, where he developed theories of polymer phase and conformational behavior, stimuli responsive polymers, and polyelectrolytes. Earlier in his career, he held internships in several industrial and academic research labs, with work including biomedical device design and fabrication, biocompatible polymer synthesis and reactor design, device testing, and thin film fluid dynamics simulation via finite difference methods.

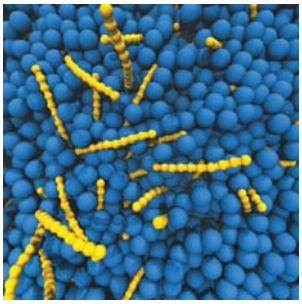
Awards/Accomplishments:

- Lead PI on $1M research grant from W. M. Keck Foundation
- National Research Council Postdoctoral Research Fellowship, (2010-2011)
- Finalist, Frank J. Padden Jr. Award for Excellence in Polymer Physics Graduate Research, (2009)
- NSF Graduate Research Fellowship Honorable Mention, (2005-2006)

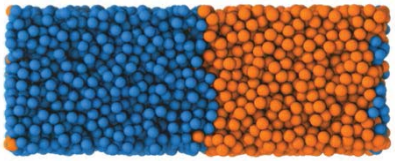
Research Interests:

Simmons' group employs theory, molecular simulation, and evolutionary optimization methods to advance the rational design of polymers and glass-forming materials with targeted dynamic, mechanical, and transport properties. Specific focus areas include:

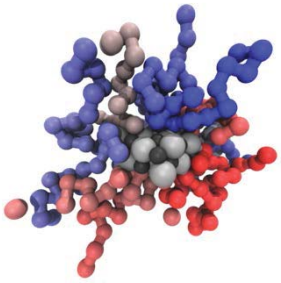
Evolving advanced polymer glasses with genetic algorithms



Developing structure/property relations for advanced additives



Advancing computational design of block and nanostructured polymers



Providing computational insights into ionomer and elastomer dynamic and mechanical properties

Industrial Sector Focus:

Polymers and processing – design of additives and polymer structural modifications for improved processability, thermal behavior, and mechanical and transport properties

Auto, aero, defense, and nanotech – rational design and structure/property relations for improved material toughness, performance, and weight

Energy and environment – charge-containing polymers for use in membranes, reduced-weight materials for energy efficiency, block-copolymers with controlled transport properties for use in membranes

Unique Laboratory Capabilities:

- High-throughput, rapid simulation of polymer dynamics, mechanical properties, and glass formation behavior
- Global optimization and design methods integrating simulation and experiment
- Dedicated access to state of the art high-performance computing resources

Recent Publications:

1. Lang, R. J., Merling, W. L., and Simmons, D. S., "Combined dependence of nanoconfined Tg on interfacial energy and softness of confinement." ACS Macro Letters 3 (2014): 758-762.
2. Marvin, M. D., Lang, R. J., and Simmons, D. S. "Nanoconfinement Effects on the Fragility of Glass Formation of a Model Freestanding Polymer Film." Soft Matter (communication) 10, no 18 (2014): 3166-3170.