The University at Buffalo Department of
Chemical and Biological Engineering
Presents

The 18th Annual Graduate Student Research Symposium

"Using High Throughput Computation to Accelerate Development of Materials for Scalable Energy Technologies"

David S. Sholl

School of Chemical &
Biomolecular Engineering

Georgia Institute of Technology,
Atlanta

Friday, September 25, 2015
Center for the Arts
UB Amherst Campus

Student Lectures 1:00 p.m.
Keynote Presentation 2:00 p.m.
Screening Room

Student Poster Competition and
Alumni/Student Mixer 3:30-5:00 p.m.
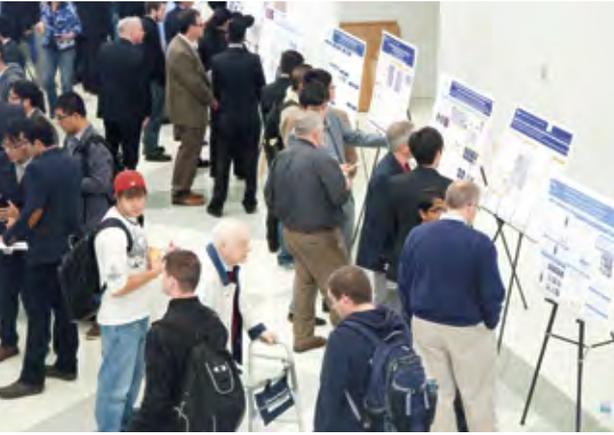**Main Stage**

RSVP cbe-chair@buffalo.edu

The School of Engineering and Applied Sciences

The UB Department of Chemical and Biological Engineering

Graduate Student Research Symposium

Over the years the UB CBE Graduate Student Research Symposium has evolved into an exciting, comprehensive event that showcases the high quality, multidisciplinary research that is conducted in our department, and spans diverse areas such as molecular engineering of novel materials, nanotechnology, bioengineering, and molecular modeling. Every year our faculty and graduate students welcome the opportunity to present their work to their peers from CBE, other UB departments, our alumni, and representatives from local business. The Symposium has grown in ambition and scale, featuring over 50 posters, two lectures from senior graduate students, and a keynote lecture from an accomplished colleague. This year we are particularly pleased to welcome Dr. David S. Sholl from the Georgia Institute of Technology. Our Symposium will include a wine, beer, and hors d'oeuvres reception to honor our alumni and guests.

CBE is proud to present our 2015 PhD candidate speakers:

- **Mahmoud Kamal Ahmadi:** "Biosynthetic Engineering and Green Manufacturing Applications for the Nonribosomal Peptide-Polyketide Siderophore Yersiniabactin"
- **Mohammad Ghasemi**: "Dissolution of Semicrystalline Polymers: Insights for Efficient Biomass Utilization Obtained by Phenomenological Modeling"

The UB Department of Chemical and Biological Engineering

This Symposium is a collaborative effort supported in part by the CBE Graduate Student Association, Praxair, Thermo Fisher Scientific, the UB CBE Advisory Board, our graduate student speakers, CBE faculty, and various colleagues in and around UB who serve as judges for the all-important student poster competition. Many thanks to all our graduate students who work so hard on their research, and for their excellent poster and oral presentations during the symposium. Special thanks to our corporate sponsors Praxair and Thermo Fisher Scientific. Ultimately, this Symposium is a showcase for the excellence that we strive for in our scholarship and graduate education. We look forward to many more years of this celebration of our research accomplishments.

www.cbe.buffalo.edu

"Using High Throughput Computation to Accelerate Development of Materials for Scalable Energy Technologies"

David S. Sholl

Georgia Institute of Technology, Atlanta

Abstract:

Computational modeling of materials can be a powerful complement to experimental methods when models with useful levels of predictive ability can be deployed more rapidly than experiments. Achieving this goal involves judicious choices about the level of modeling that is used and the key physical properties of the materials of interest that control performance in practical applications. I will discuss two examples of using high throughput computations to identify new materials for scalable energy applications: the use of metal-organic frameworks in membranes and gas storage and the selection of metal hydrides for high temperature nuclear applications. These examples highlight the challenges of generating sufficiently comprehensive material libraries and the potential advantages and difficulties of using computational methods to examine large libraries of materials.
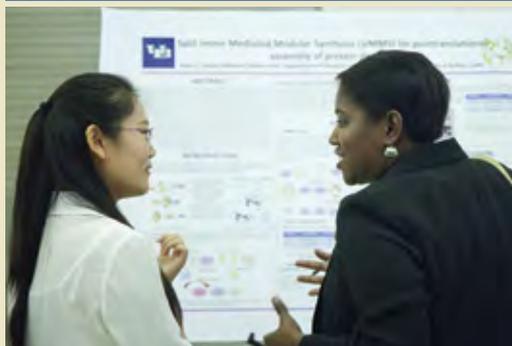
About David Sholl:

David Sholl is the School Chair of Chemical & Biomolecular Engineering at Georgia Tech, where he is also the Michael E. Tennenbaum Family Chair and GRA Eminent Scholar in Energy Sustainability. David's research uses computational materials modeling to accelerate development of new materials for energy-related applications, including generation and storage of gaseous and liquid fuels and carbon dioxide mitigation. He has published over 260 peer-reviewed papers. He has also written a textbook on Density Functional Theory, a quantum chemistry method that is widely applied through the physical sciences and engineering. David is a Senior Editor of the ACS journal Langmuir.

More information on David's research group is available from www.chbe.gatech.edu/sholl.

Join us for the 2015 18th Annual Graduate Student Research Symposium

Friday, September 25th at 1:00 p.m.

Friday, September 25th at 3:30 p.m.

UB CBE POSTER COMPETITION AND ALUMNI/STUDENT MIXER

3:30-5:00 p.m. Center for the Arts

• Meet David Sholl • Learn what's new • Connect with your colleagues •

• Wine • beer • soft drinks • hors d'oeuvres •

R.S.V.P. cbe-chair@buffalo.edu or call 716.645.1174

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Reconnect with UB CBE:

- Send us your "Faces of CBE" profile
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- Like us on Facebook and LinkedIn
- Sign up for the CBE monthly e-bulletin

- COME TO AN EVENT!
  NEXT UP: SEPTEMBER 25TH, UB CBE POSTER COMPETITION AND ALUMNI/STUDENT MIXER

Contact Us:

- To R.S.V.P. and learn more about how you can reconnect, write to: cbe-chair@buffalo.edu
  call: 716.645.1174
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