

Heather Beth Mayes

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Education

- 2010–Present **Northwestern University, Evanston, IL**
PhD Candidate, Department of Chemical and Biological Engineering
Advisors: Dr. Linda J. Broadbelt (Northwestern) and Dr. Gregg T. Beckham (NREL)
- Dissertation: Harnessing computational chemistry to uncover the molecular mechanisms that underlie thermochemical and enzymatic cellulose decomposition
 - Department of Energy (DOE) Computational Science Graduate Fellow (CSGF)
 - Management for Scientists and Engineers, Kellogg School of Management
- 2004–2007 **University of Illinois at Chicago, Chicago, IL**
Bachelor of Science in Chemical Engineering, magna cum laude (institutional GPA 4.0/4.0)
- Harvard University, Cambridge, MA**
Studied writing, Spanish, and comparative religion
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Professional Experience

- Spring 2014 **Northwestern University, Evanston, IL**
Teaching apprentice for upper-level undergraduate introduction to statistical mechanics
- Additionally: earned Searle Center for Teaching Excellence's Teaching Certificate; course design project selected to be featured as a "great" example for future participants
 - Previously: teaching assistant and guest lecturer for chemical engineering senior design
- Spring 2012 **National Renewable Energy Laboratory, Golden, CO**
Intern, National Bioenergy Center
- CSGF Practicum Project: Performed a Car-Parrinello Molecular Dynamics (CPMD) study of lignol radical recombination to elucidate lignin biosynthesis
- 2007–2010, **Jacobs Consultancy, Chicago, IL**
Summer 2006 *Consultant 2007–2010, Intern for summer 2006*
- Performed process modeling, kinetic modeling, linear programming, life cycle assessment, and risk analysis to help companies make their processes safer, more efficient, and more cost-effective
- Summer 2005 **Argonne National Laboratory, Argonne, IL**
DOE Summer Undergraduate Laboratory Intern (SULI), Chemical Engineering Division
- Supported the Advanced Fuel Cycle Initiative and Reduced Enrichment for Research and Test Reactors Program
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Selected Honors

- 2014 American Institute of Chemical Engineers (AIChE) Computational Molecular Science and Engineering Forum (CoMSEF) Graduate Student Award
- 2014 Featured on the cover of and profiled in the 2014 issue of *DEIXIS*, the annual publication of the DOE Computational Science Graduate Fellowship
(<https://www.krellinst.org/csgf/outreach/deixis-magazine>)

- 2014 Northwestern University Department of Chemical and Biological Engineering Distinguished Graduate Researcher Award
- 2014 Kemin Travel Award to the 2015 Spring American Chemical Society (ACS) Meeting
- 2014 AIChE Women's Initiatives Committee Travel Grant
- 2014 AIChE Catalysis and Reaction Engineering (CRE) Division Travel Award
- 2014 ACS Chemical Computing Group Research Excellence Award (COMP Division)
- 2014 Invited presenter, University of Washington's Distinguished Young Scholars Seminar series; voted 2nd place speaker
- 2014 Society of Women Engineers (SWE) Chicago Outreach Award
- 2014 SWE Chicago SWEetheart of the Month
- 2013 Selected to participate in the 63rd Lindau Nobel Laureate Meeting
- 2013 Chosen to debate biofuels with Laureates Steven Chu and Hartmut Michel in a *Nature* video (<http://www.mediatheque.lindau-nobel.org/videos/31206/2013-3>)
- 2013 SWE Chicago Key Contributor Award
- 2012 SWE Chicago SWEetheart of the Month
- 2012 NSF Pan-American Advanced Studies Institutes Program Award to attend a Multiscale Modeling and Simulation workshop in Montevideo, Uruguay
- 2011 NSF Partnerships for International Research and Education Award to attend "Energy and Materials from the Sun," Netherlands
- 2011–2015 DOE Computational Science Graduate Fellowship (CSGF)
- 2011–2015 ARCS Foundation Scholar
- 2007 University of Illinois Alumni Association Student Leadership Award
- 2006 Nagel Scholarship from Tau Beta Pi
- 2006 Women in Science and Engineering (WISE) Mentor of the Year Award
- 2006 Leonard Kotin Memorial Award for Physical Chemistry
- 2006 Society of Women Engineers DuPont Scholarship
- 2006 College of Engineering Caterpillar Scholar
- 2005 Inder P. Batra Physics Undergraduate Award

Publications

Peer-Reviewed: * Denotes equal contribution

10. **Mayes, H. B.**; Knott, B. C.; Crowley, M. F.; Götz, A. W.; Ståhlberg, J.; Broadbelt, L. J.; Beckham, G. T. "Who's on Base? The catalytic cycle of the inverting glycoside hydrolase *T. reesei* Cel6A." In preparation.
9. **Mayes, H. B.**; Broadbelt, L. J.; Beckham, G. T. "Sugar Puckering with *Ab Initio*, DFT, and Semi-Empirical Methods." In preparation.
8. Zhou, X.; Nolte, M. W.; **Mayes, H. B.**; Shanks, B. H.; Broadbelt, L. J. "Experimental study and mechanistic modeling of fast pyrolysis of glucose-based carbohydrates in the presence of NaCl." *Energy Environ. Sci.* In review.
7. Payne, C. M.*; Knott, B. C.*; **Mayes, H. B.***; Hansson, H.; Himmel, M. E.; Sandgren, M.; Ståhlberg, J.; Beckham, G. T. "Fungal Cellulases." *Chem. Rev.* In revision.
6. **Mayes, H. B.**; Nolte, M. W.; Beckham, G. T.; Shanks, B. H.; Broadbelt, L. J. "Salty Alpha-Bet(a) of Glucose Pyrolysis: Computational and Experimental Investigations of Key Reactions Under the Influence of Na⁺ Reveal Implications for Cellulose Pyrolysis." *ACS Catal.* In press.
5. Zhou, X.; Nolte, M. W.; **Mayes, H. B.**; Shanks, B. H.; Broadbelt, L. J. "Experimental and Mechanistic Modeling of Fast Pyrolysis of Neat Glucose-Based Carbohydrates. 1.

Experiments and Development of a Mechanistic Model.” *Ind. Eng. Chem. Res.*, **2014**, *53*, 13274–13289. *ACS Editors’ Choice article*.

4. **Mayes, H. B.**; Nolte, M. W.; Beckham, G. T.; Shanks, B. H.; Broadbelt, L. J. “The Alpha-Bet(a) of Glucose Pyrolysis: Computational and Experimental Investigations of Glucose Anomers Reveal Implications for Cellulose Pyrolysis.” *ACS Sustainable Chem. Eng.*, **2014**, *2*, 1461-1473. *ACS Editors’ Choice article*.
3. **Mayes, H. B.**; Tian, J.; Nolte, M. W.; Shanks, B. H.; Beckham, G. T.; Gnanakaran, S.; Broadbelt, L. J. “Sodium Ion Interactions with Aqueous Glucose: Insights from Quantum Mechanics, Molecular Dynamics, and Experiment.” *J. Phys. Chem. B*, **2014**, *118*, 1990–2000. *Featured on cover*.
2. **Mayes, H. B.**; Broadbelt, L. J.; Beckham, G. T. “How Sugars Pucker: Electronic Structure Calculations Map the Kinetic Landscape of Five Biologically Paramount Monosaccharides and Their Implications for Enzymatic Catalysis.” *J. Am. Chem. Soc.*, **2014**, *136*, 1008–1022.
1. **Mayes, H. B.**; Broadbelt, L. J. “Unraveling the Reactions that Unravel Cellulose.” *J. Phys. Chem. A*, **2012**, *116*, 7098–7106. *34 citations*.

Commentary: 1. **Mayes, H. B.***; Sheehan, S. W.*; Dotan, H.* “Energy: Fueling the Future.” *Nature*, **2013**, *502*, S60–S61.

Presentations

- Invited:**
7. **Mayes, H. B.**; Zhou, X.; Beckham, G. T.; Broadbelt, L. J. “Charting Elementary Steps in the Cellulose Pyrolysis Reaction Network.” Computational Pyrolysis & Upgrading of Bio-Oils, ACS Spring 2015 National Meeting & Exposition (Denver, CO; March 2015).
 6. **Mayes, H. B.**; Beckham, G. T.; Broadbelt, L. J. “The Elementary Steps of Cellulose Pyrolysis Map a Road to Renewable Fuels.” Distinguished Graduate Researcher Presentation, Northwestern University Department of Chemical and Biological Engineering Annual Retreat (Glencoe, IL; September 2014).
 5. **Mayes, H. B.**; Broadbelt, L. J.; Beckham, G.T. “Why Pucker, Sugar? Computational Chemistry Investigations into Carbohydrate Ring Distortion for Enzymatic Action.” Chemical Computing Group Excellence Award for Graduate Students, ACS Fall 2014 National Meeting & Exposition (San Francisco, CA; August 2014).
 4. **Mayes, H. B.**; Beckham, G.T.; Broadbelt, L. J. “Discerning Mechanisms in the Cellulose Pyrolysis Reaction Network.” University of Washington Distinguished Young Seminar Series (Seattle, WA; August 2014).
 3. **Mayes, H. B.**; Beckham, G.T.; Broadbelt, L. J. “New Insights into Cellulose Pyrolysis Reaction Kinetics.” 6th Annual AIChE Midwest Regional Conference (Chicago, IL; March 2014).
 2. **Mayes, H. B.**; Beckham, G. T.; Broadbelt, L. J. “Revealing Reactions in Cellulose Pyrolysis.” Plenary Session: Computational Molecular Science and Engineering Forum, PASI Poster Award Recognition, AIChE Annual Meeting (San Francisco, CA; November 2013).
 1. **Mayes, H. B.**; Broadbelt, L. J.; Beckham, G. T. “Mapping Sugars Along Catalytic Itineraries: A Case Study in Exploring Multi-Dimensional Landscapes.” DOE Computational Science Graduate Fellowship Program Showcase, SIAM Conference on Computational Science and Engineering (Boston, MA; February 2013).

- Contributed:**
12. **Mayes, H. B.**; Zhou, X.; Beckham, G.T.; Broadbelt, L. J. “Discerning and Modeling Reaction Mechanisms in Cellulose Pyrolysis.” 2014 AIChE Annual Meeting (Atlanta, GA; November 2014).
 11. **Mayes, H. B.**; Beckham, G. T.; Broadbelt, L. J. “Why Pucker, Sugar? Computational Chemistry Investigations into Carbohydrate Ring Distortion for Enzymatic Action.” 2014 AIChE Annual Meeting (Atlanta, GA; November 2014).
 10. **Mayes, H. B.**; Beckham, G. T.; Broadbelt, L. J. “Discerning Mechanisms in the Cellulose Pyrolysis Reaction Network.” Industrial and Engineering Chemistry Division Graduate Student Award Symposium, ACS Fall 2014 National Meeting & Exposition (San Francisco, CA; August 2014).
 9. **Mayes, H. B.**; Beckham, G. T.; Broadbelt, L. J. “Thermodynamics and Kinetics of Carbohydrate Ring Puckering.” Gordon Research Seminar and Gordon Research Conference on Cellulosomes, Cellulases and Other Carbohydrate Modifying Enzymes (Andover, NH; August 2013).
 8. **Mayes, H. B.** “5 Things You Can Do to Reach Out to Underrepresented Groups in STEM.” CSGF +1 (Washington, DC; July 2013).
 7. **Mayes, H. B.**; Broadbelt, L. J.; Beckham, G. T. “Elucidating Enzymatic Routes to Biomass Deconstruction: Quantifying Method Accuracy for Mapping Glycosidic Hydrolase Catalytic Itineraries.” PASI workshop (Montevideo, Uruguay; September 2012). *Best poster award.*
 6. **Mayes, H. B.**; Zhang, J.; Shanks, B. H.; Broadbelt, L. J. “Sodium-Mediated Glucose Pyrolysis: Experimental Results and Mechanistic Dehydration Study.” ACS Fall 2012 National Meeting & Exposition (Philadelphia, PA; August 2012).
 5. **Mayes, H. B.**; Broadbelt, L. J. “Unraveling the Reactions which Unravel Cellulose.” ACS Spring 2012 National Meeting & Exposition (San Diego, CA; March 2012).
 4. **Mayes, H. B.**; Vinu, R.; Broadbelt, L. J. “*Ab Initio* Calculations to Determine Cellulose Fast Pyrolysis Reaction Mechanisms.” tcbiomass2011 (Chicago, IL; Sept. 2011).
 3. **Mayes, H. B.**; Ravikrishnan, V.; and Broadbelt L. J. "Computational Chemistry to Elucidate Cellulose Fast Pyrolysis Reaction Mechanisms." Fall Creek Falls Conference on Computing and Computational Sciences (Gatlinburg, TN; Sept. 2011).
 2. Stepinski, D. C.; **Mayes, H. B.**; Bakel, A. J.; Leyva, A.; Gelis, A. V.; Bond, A. H.; and Vandegrift, G. F. “Efficient Separation of Mo-99 from Low-Enriched Uranium Using Inorganic Sorbents.” Fourteenth Symposium on Separation Science and Technology for Energy Applications (Gatlinburg, TN; Oct. 2005).
 1. Bakel, A. J.; Stepinski D. C.; Vandegrift, G. F.; Leyva, A.; Gelis, A. V.; Bond, A. H.; **Mayes H. B.** “Progress in Technology Development for Conversion of ⁹⁹Mo Production—BATAN’s (Indonesia) Conversion Program, Progress in the CNEA (Argentina) LEU Foil/Base-Side Process, and Development of Inorganic Sorbents for ⁹⁹Mo Production.” The RERTR-2005 International Meeting on Reduced Enrichment for Research and Test Reactors (Boston, MA; Nov. 2005).

Professional Memberships

- American Institute of Chemical Engineers
- Society of Women Engineers
- American Chemical Society
- American Association for the Advancement of Science

Service

Northwestern University

- 2013, 2014 Speaker and co-organizer of graduate fellowship panels for first-year graduate students and upper-class undergraduates
- 2011–2014 Tour lead for annual Career Day for Girls
- 2014 Invited SWE Industry Panel speaker
- 2011–2014 Pen pal for “Letters to a Pre-Scientist”
- 2013 Invited speaker for junior high school student visit to McCormick School of Engineering
- 2013 McCormick Graduate Leadership Committee Science Pentathlon volunteer
- 2012 Served on departmental committee on information flow
- 2011 Departmental annual retreat planning committee

Society of Women Engineers

- 2013, 2014 Lead for Parents and Educators Program (PEP) of the signature outreach event (*Invent It. Build It.*) at the annual national meeting
- 2014–Present Chicago Regional Section Representative
- 2014 Invited speaker for “Voices from the Field” outreach webinar series
- 2013–Present Collegiate Counselor to Northwestern University SWE
- 2012 Invited panelist for the PEP at *Invent It. Build It.*
- 2013–2014 Chicago Regional Section Corresponding Secretary
- 2012–2013 Chicago Regional Section Treasurer
- 2011–Present Outreach volunteer (including mentoring) with the Northwestern and Chicago sections
- 2009–2013 Chicago Regional Section Webmaster

American Institute of Chemical Engineers

- 2007–2010 Webmaster for the Chicago professional section
- 2007–2008 Secretary for the Chicago professional section