

# Alex Dickson

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## CONTACT INFORMATION

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East Lansing, MI 48824  
USA

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## GOALS

**To apply novel tools and techniques from molecular simulation to biological systems relevant to human disease.**

## SPECIFIC AREAS OF INTEREST

MD-driven drug development, biological systems modeling, network analysis, chaperone-mediated folding, developing new methods for computer simulation of molecular systems, systems driven out of equilibrium, dynamical phase transitions

## EDUCATION AND EXPERIENCE

**Michigan State University**, East Lansing, MI

**Assistant Professor**, Department of Biochemistry and Molecular Biology, September 2015–Present

- Joint appointment with the Department of Computational Mathematics, Science and Engineering

**University of Michigan**, Ann Arbor, MI

**Postdoctoral Fellow**, Department of Chemistry, September 2011–August 2015

Primary Mentor: Charles L. Brooks, III

- Studied relative path probabilities to elucidate mechanisms of chaperone activity in *E. coli*
- Developed analysis techniques (“hub scores”) to elucidate high-level behaviors in complex networks
- Created and applied new custom enhanced sampling methods to explore new areas of configuration space in high-dimensional order parameter spaces (“WEExplore”)
- Elucidated mechanisms of interaction for the intrinsically disordered chaperone HdeA

**University of Chicago**, Chicago, IL

**Ph.D.**, Department of Chemistry, July 2011

Dissertation Topic: *“Enhanced sampling methods for nonequilibrium systems”*

Advisor: Aaron R. Dinner

- Developed enhanced sampling methods to study systems driven out of equilibrium (“nonequilibrium umbrella sampling”)
- Ran massively parallel simulations on supercomputing architectures
- Studied dynamical phase transitions using large deviation theory

**M.S.**, Chemistry, May 2007

**University of Toronto**, Ontario, Canada

**Hon. B. Sc.**, Chemical Physics (Minor: Mathematics), May 2006

Thesis: *“The effect of trajectory accuracy on statistical distributions in chaotic systems”*

## PERSONAL INFORMATION

I am a dual Canadian-American citizen.

I am an ACS member 30919152, and a member of ACS COMP since 2015.

[\*] = corresponding author

- [1] Lotz SD and **Dickson A\*** (In press) Wepy: A Flexible Software Framework for Simulating Rare Events with Weighted Ensemble Resampling. *ACS Omega*.
- [2] Roussey NM and **Dickson A\*** (2020) Enhanced Jarzynski Free Energy Calculations using Weighted Ensemble. *J. Chem. Phys.* 153:134116.
- [3] Hall R, Dixon T, **Dickson A\*** (2020) On Calculating Free Energy Using Ensembles of Transition Paths. *Frontiers in Molecular Biosciences* 7:106.
- [4] Rizzi A, Jensen T, Slochower DR, Aldeghi M, Gapsys V, Ntekoumes D, Bosisio S, Papadourakis M, Henriksen NM, de Groot BL, Cournia Z, **Dickson A**, Michel J, Gilson MK, Shirts MR, Mobley DM\* and Chodera JD\* (2020) The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. *Journal of Computer Aided Molecular Design* 34:601-633.
- [5] Bogetti AT, Mostofian B, **Dickson A**, Pratt AJ, Saglam AS, Harrison PO, Adelman JL, Dudek M, Torrillo PA, DeGrave AJ, Adhikari U, Zwier MC, Zuckerman DM\* and Chong LT\* (2019) A Suite of Tutorials for the WESTPA Rare-Events Sampling Software [Article v1.0]. *Living Journal of Computational Molecular Science* 1(2):10607.
- [6] Donyapour N, Roussey NM and **Dickson A\*** (2019) REVO: Resampling of Ensembles by Variation Optimization. *Journal of Chemical Physics* 150:244112.
- [7] Liu Y, Hickey DP, Minter SD, **Dickson A\*** and Barton SC\* (2019) Markov-State Transition Path Analysis of Electrostatic Channeling. *Journal of Physical Chemistry C* 123: 15284-15292. **\*\*Cover article\*\***
- [8] Kirberger SE, Ycas PD, Johnson JA, Chen C, Ciccone M, Lu RWW, Urlick AK, Zahid H, Shi K, Aihara H, McAllister SD, Kashani-Sabet M, Shi J, **Dickson A**, dos Santos CO\* and Pomerantz WCK\* (2019) Selectivity, ligand deconstruction, and cellular activity analysis of a BPTF bromodomain inhibitor. *Organic & Biomolecular Chemistry* 17: 2020-2027.
- [9] Bai N, Roder H, **Dickson A** and Karanicolas J\* (2019) Isothermal Analysis of ThermoFluor Data can readily provide Quantitative Binding Affinities. *Scientific Reports* 9:2650.
- [10] **Dickson A\*** (2018) Mapping the Ligand Binding Landscape. *Biophysical Journal* 115:1707-1719.
- [11] Dixon T, Lotz SD, **Dickson A\*** (2018) Predicting Ligand Binding Affinity Using On- and Off-Rates for the SAMPL6 SAMPLing Challenge. *Journal of Computer-Aided Molecular Design* 32(10):1001-1012 **\*\*Cover article\*\***
- [12] Zeng X, Uyar A, Sui D, Donyapour N, Wu D, **Dickson A\***, Hu J\* (2018) Structural Insights Into Lethal Contractural Syndrome Type 3 (LCCS3) Caused by a Missense Mutation of PIP5Ky. *Biochemical Journal* 475: 2257-2269.

- [13] Lotz SD and **Dickson A\*** (2018) Unbiased Molecular Dynamics of 11 min Timescale Drug Unbinding Reveals Transition State Stabilizing Interactions. *Journal of the American Chemical Society* 140: 618-628.
- [14] Wood RJ, Ormsby AR, Radwan M, Cox D, Sharma A, Vopel T, Ebbinghaus S, Oliveberg M, Reid GE, **Dickson A**, Hatters DM\* (2018) A Biosensor-Based Framework to Measure Latent Proteostasis Capacity. *Nature Communications* 9:287.
- [15] Uyar A, Karamyan VT and **Dickson A\*** (2018) Long-Range Changes in Neurolysin Dynamics Upon Inhibitor Binding. *Journal of Chemical Theory and Computation* 14: 444-452.
- [16] **Dickson A\***, Tiwary P and Vashisth H (2017) Kinetics of Ligand Binding Through Advanced Computational Approaches: A Review. *Current Topics in Medicinal Chemistry* 17: 2626-2641.
- [17] **Dickson A\***, Lotz SD (2017) Multiple Unbinding Pathways and Ligand-Induced Destabilization Revealed by WExplore and Conformation Space Networks. *Biophysical Journal* 112: 620-629.
- [18] **Dickson A\***, Bailey CT and Karanicolas J (2016) Optimal Allosteric Stabilization Sites Using Contact Stabilization Analysis. *Journal of Computational Chemistry* 38: 1138-1146.
- [19] **Dickson A\***, Lotz SD (2016) Ligand Release Pathways Obtained with WExplore: Residence Times and Mechanisms. *Journal of Physical Chemistry B* 120: 5377-5385.

#### PUBLICATIONS IN SUBMISSION

[\*] = corresponding author

- [1] Dixon T, Uyar A, Ferguson-Miller S, **Dickson A\*** (2020) Membrane-mediated ligand unbinding of the PK-11195 ligand from the translocator protein (TSPO). *bioRxiv* DOI:<https://doi.org/10.1101/2020.01.21.914127> .

#### PUBLICATIONS WITH [\*] = corresponding author FORMER MENTORS

- [1] Salmon L, Ahlstrom LS, Horowitz S, **Dickson A**, Brooks III CL\*, Bardwell, JCA\* (2016) Capturing a dynamic chaperone-substrate interaction using NMR-informed molecular modeling. *Journal of the American Chemical Society* 138: 9826-9839.
- [2] **Dickson A**, Ahlstrom LS, Brooks III CL\* (2015) Coupled Folding and Binding with 2D Window-Exchange Umbrella Sampling. *Journal of Computational Chemistry* 37: 587-594. **\*\*Cover article\*\***
- [3] Ahlstrom LS, Law S, **Dickson A**, Brooks III CL\* (2015) Multiscale Modeling of a Conditionally Disordered pH-Sensing Chaperone *Journal of Molecular Biology* 427: 1670-1680.
- [4] Laricheva E, Goh G, **Dickson A**, Brooks III CL\* (2015) pH-Dependent Transient Conformational States Control Optical Properties in Cyan Fluorescent Protein *Journal of the American Chemical Society* 137: 2892-2900.

- [5] **Dickson A**, Mustoe AM, Salmon L, Brooks III CL\* (2014) Efficient In-Silico Exploration of RNA Interhelical Conformations Using Euler Angles and WExplore. *Nucleic Acids Research* 42: 97-110.
- [6] **Dickson A**, Brooks III CL\* (2014) WExplore: Hierarchical exploration of high dimensional spaces using the weighted ensemble algorithm. *Journal of Physical Chemistry B* 118: 3532-3542. **\*\*Cover article\*\***
- [7] **Dickson A**, Brooks III CL\* (2013) Quantifying chaperone-mediated transitions in the proteostasis network of E. coli. *PLoS Computational Biology* 9: e1003324.
- [8] **Dickson A**, Brooks III CL\* (2013) Native states of fast-folding proteins are kinetic traps. *Journal of the American Chemical Society* 135: 4729-4734.
- [9] Ahlstrom LS, **Dickson A**, Brooks III CL\* (2013) Binding and Folding of the Small Bacterial Chaperone HdeA. *Journal of Physical Chemistry B* 117: 13219-13225.
- [10] **Dickson A**, Brooks III CL\* (2012) Quantifying hub-like behavior in protein folding networks. *Journal of Chemical Theory and Computation* 8: 3044-3052.
- [11] **Dickson A**, Tabei SMA, Dinner AR\* (2011) Entrainment of a driven oscillator as a dynamical phase transition. *Physical Review E* 84: 061134.
- [12] **Dickson A**, Maienschein-Cline M, Tovo-Dwyer A, Hammond JR, Dinner AR\* (2011) Flow-dependent unfolding and refolding of an RNA by nonequilibrium umbrella sampling. *Journal of Chemical Theory and Computation* 7: 2710-2720.
- [13] **Dickson A**, Nasto A, Dinner AR\* (2010) Incorporating friction and collective shear moves into a lattice gas. *Physical Review E* 81: 051111.
- [14] **Dickson A**, Dinner AR\* (2010) Enhanced sampling of nonequilibrium steady states. *Annual Reviews of Physical Chemistry* 61: 441-459.
- [15] **Dickson A**, Warmflash A, Dinner AR\* (2009) Separating forward and backward pathways in nonequilibrium umbrella sampling. *Journal of Chemical Physics* 131: 154104.
- [16] **Dickson A**, Warmflash A, Dinner AR\* (2009) Nonequilibrium umbrella sampling in spaces of many order parameters. *Journal of Chemical Physics* 130: 074104.

## FUNDING

**NIH NIGMS R01 Administrative Supplement** **2019 Total:** \$124,464 USD  
*Mapping the ligand binding landscape with advanced molecular simulation methods*  
**PI:** Alex Dickson (MSU)

**NIH NIGMS R01 Grant** **2018-2022 Total:** \$1.3 M USD  
*Mapping the ligand binding landscape with advanced molecular simulation methods*  
**PI:** Alex Dickson (MSU)

**DMS/NIGMS** Research at the Interface of Bio. and Math. Sciences **2018-2022** Total: \$1.1 M USD  
*Kinetics-driven drug discovery using persistent homology, rare event molecular dynamics and experimental data*

**Lead PI:** Alex Dickson (MSU), **Co-PIs:** Guowei Wei (MSU), Kin Sing Stephen Lee (MSU)

**Human Frontiers Science Program**, Program Grant **2017-2020** Total: \$1.2 M USD  
*Defining the Capacity of Cells to Keep the Proteome Folded Over Space and Time*

**Lead PI:** Danny Hatters (U. Melbourne), **Co-PIs:** Alex Dickson (MSU), Hannah Nicholas (U. Sydney), Simon Ebbinghaus (Ruhr. Univ. Bochum)

## ARTICLES REVIEWED

I have served as a referee for articles submitted to the journals *Proceedings of the National Academy of Sciences*, *Journal of Molecular Graphics and Modelling*, *Journal of Computational Chemistry*, *Biopolymers*, *Journal of the American Chemical Society*, *Computational Biology and Chemistry*, *Frontiers in Bioengineering and Biotechnology*, *PLoS Computational Biology*, *Biophysical Journal* and *Proteins: Structure, Function and Bioinformatics*.

## PROPOSALS REVIEWED

**Panel Member**, NSF

**Ad hoc Reviewer**, NSF CAREER

**Ad hoc Reviewer**, NSF CAREER

**Ad hoc Reviewer**, NSF CAREER

**Ad hoc Reviewer**, NSF CAREER

DMS NIGMS-A, 2019.

Chemistry of Life Processes, 2019.

Chemistry of Life Processes, 2019.

Chemistry of Life Processes, 2018.

Chemical Theory, Models and Computational Methods 2018.

## TEACHING

### BMB803/805

**Spring 2020**

*Protein Structure, Design and Mechanism*, 11 lecture hours.

A series of lectures and computational laboratories on protein sequence, structure and function. Developed a final project component where students create molecular visualizations to present a molecular system to a broad audience.

### CMSE201

**Fall 2019**

*Introduction to Computational Modeling*, 60 lecture hours.

An introductory undergraduate course that teaches Python programming and computer modeling of real-world systems. Solo-taught one 70-student section.

### BMB803/805

**Spring 2019**

*Protein Structure, Design and Mechanism*, 11 lecture hours.

A series of lectures and computational laboratories on protein sequence, structure and function. Developed a final project component where students create molecular visualizations to present a molecular system to a broad audience.

### CMSE201

**Fall 2018**

*Introduction to Computational Modeling*, 60 lecture hours.

Solo-taught one 70-student section.

### CMSE201

**Fall 2017**

*Introduction to Computational Modeling*, 6 lecture hours.

Taught three sections of a guest lecture on Langevin dynamics.

### BMB961/CMSE890

**Spring 2017**

*Concepts in Protein Structure and Modeling*, 12 lecture hours.

Lectures and laboratories concerning enhanced sampling methods, clustering and kinetic modeling, and

binding free energy calculations. Co-taught with Dr. Michael Feig.

### CMSE801

Fall 2016

*Introduction to Computational Modeling*, 24 lecture hours.

Co-taught with Dr. Alexei Bazavov. Graduate course with lectures and laboratories on creating physical and computational models; programming in Python; effective visualization of data; working in teams to computationally solve scientific problems.

### NSC801

Spring 2016

*Introduction to Computational Modeling*, 24 lecture hours.

Graduate course co-taught with Dr. Mohsen Zayernouri. All course material was developed from scratch by myself and Dr. Zayernouri.

### STUDENTS MENTORED

#### Current

Dr. Arzu Uyar (Postdoctoral researcher)  
Samuel D. Lotz (Ph.D. candidate), anticipated graduation in 2020.  
Tom Dixon (Ph.D. candidate)  
Nicole Roussey (Ph.D. candidate)  
Nazanin Donyapour (Ph.D. candidate)  
James Lennon (Ph.D.)

#### Past

Thomas Diaz (M.Sc. Chemistry, 2019)  
Robert Hall (Post baccalaureate student)

### INVITED TALKS

**Online Presentation**, ACS Virtual Meeting, Fall 2020.

**Departmental Seminar**, Chemical and Biomolecular Engineering, University of California, Irvine, May 2020 (virtual)

**Departmental Seminar**, Biochemistry & Molecular Biology, University of Oklahoma, April 2020 (cancelled due to COVID-19)

**From protein folding to ligand binding: adventures with free energies**, ACS Meeting, March 2020 (cancelled due to COVID-19)

**Biophysics Seminar**, University of Michigan, September 2019.

**Free energy calculations: Entering the fourth decade of adventure in chemistry and biophysics**, Santa Fe, June 2019.

**Sampling conformations and pathways in biomolecular systems**, ACS Meeting, April 2019.

**Bioinformatics Cluster Meeting**, University of Rochester, April 2019.

**Physics Seminar**, Oakland University, December 2018.

**Chemistry Seminar**, William Paterson University, October 2018.

**WEExplore lecture @ WESTPA Workshop**, University of Pittsburgh, August 2018.

**WEExplore plugin tutorial @ WESTPA Workshop**, University of Pittsburgh, August 2018.

**Mid-Atlantic Comp Chem Meeting** (via web) with Merck, GlaxoSmithKline, Bristol-Myers Squibb, and Pfizer, March 2018.

**Seminar**, Department of Computational & Systems Biology, University of Pittsburgh, September 2017.

**Modeling & Measuring Protein-Ligand Kinetics & Residence Times**, ACS Meeting, August 2017.

**Physical Chemistry Seminar**, Michigan State University, September 2016.

**Charlie Brooks 60th Birthday Celebration**, ACS Meeting, March 2016.

**Pharmacology & Toxicology Seminar**, Michigan State University, February 2016.

**Computer Science and Engineering Seminar**, Michigan State University, October 2015.

**WESTPA Workshop**, University of Pittsburgh, July 2015.

**University of British Columbia, Okanagan Campus**, Department of Chemistry, February 2015.

**Michigan State University**, Department of Biochemistry and Molecular Biology, February 2015.  
**IUPUI**, Department of Chemistry, February 2015.  
**University of Texas, El Paso**, Department of Chemistry, December 2014.  
**University at Buffalo**, Department of Chemistry, November 2014.  
**Protein Folding Consortium** in Ann Arbor, MI, June 2014.  
**Washington University St. Louis**, Department of Biochemistry and Molecular Biophysics, March 2014.  
**Protein Folding Consortium Workshop** in Berkeley, June 2013.  
**After Mini Mini** for path sampling methods in Berkeley, Jan 2010.  
**Multiscale Materials Modeling** in Tallahassee, Oct 2008.

CONTRIBUTED  
TALKS AND  
POSTER SESSIONS

**ACS Meeting** (Poster), San Diego, August 2019.  
**Biophysical Society Meeting** (Talk), Baltimore, March 2019.  
**Free Energy Methods, Kinetics and Markov State Models in Drug Design** (Poster), Cambridge, May 2018.  
**Binding Kinetics: Time is of the Essence** (Poster), Berlin, October 2017.  
**ACS Meeting** (Talk), Washington DC, August 2017.  
**ACS Meeting** (Talk), San Francisco, April 2017.  
**Biophysical Society Meeting** (Talk), Los Angeles, February 2016.  
**q-bio Winter Meeting** in Hawaii (Poster), February 2014.

HONORS AND  
AWARDS

**OpenEye Outstanding Junior Faculty Award**, American Chemical Society, COMP Division, 2019.  
**Elizabeth R. Norton Prize for Excellence in Research in Chemistry**, University of Chicago, 2010.  
**Postgraduate Scholarship**, Natural Sciences and Engineering Research Council of Canada (NSERC), 2007-2011.  
**Freud Scholar Fellowship**, University of Chicago, 2006.  
**Undergraduate Student Research Award**, NSERC, 2005.  
**Undergraduate Student Research Award**, NSERC, 2004.  
**Susan C. Gollop and William G. Gollop Scholarship in Chemistry**, University of Toronto, 2002-2003.

SERVICE

**Presider**, American Chemical Society Meeting: Sampling Conformations & Pathways in Biomolecular Systems, Orlando, April 2019.  
**Session chair**, Biophysical Society Meeting: Protein-Small Molecular Interactions, Baltimore, March 2019.  
**Organizer**, Midwest Computational Chemistry Conference, East Lansing, MI, June 2017.  
**Organizer**, BMB Departmental Retreat, East Lansing, MI, September 2016.  
**Organizer**, Computational Biology Symposium, Ann Arbor, MI, September 2016.  
**Session chair**, Biophysical Society Meeting: Protein-Small Molecule Interactions, Los Angeles, February 2016.  
**Session chair**, Gordon Research Seminar: Computational Chemistry, July 2014.

COMMUNITY  
OUTREACH

**MSU Science Festival**, Abrams Planetarium **2016-2019**  
*Small Molecules on the Big Screen* (2019)  
*Small Molecules on the Big Screen* (2018)  
*Small Molecules on the Big Screen* (2017)  
*What Happens to Molecules When You Turn Up the Heat?* (2016)  
 40-min talks with dome-formatted molecular visualizations designed to appeal to younger audiences.  
 Topics include: phase transitions (ice → water → steam), DNA synthesis, destabilizing protein mutations, molecular definition of temperature.



<b>MSU Grandparents' University</b> <i>How Do Molecules Find Their Perfect Fit?</i> Taught two 1.5 hr lectures for children and their grandparents, employing 3D printed models of proteins to demonstrate key principles of molecular interaction. Topics included: assembly of viral capsids, molecular recognition, protein conformational change.	<b>2016-2017</b>
<b>Faculty Advisory Committee, BMB, Michigan State University</b> <i>Member</i>	<b>2019-Present</b>
<b>Organizing committee, Science at the Edge, Michigan State University</b> <i>Member</i>	<b>2019-Present</b>
<b>Computer committee, BMB, Michigan State University</b> <i>Chair</i>	<b>2018-Present</b>
<b>Undergraduate Studies Committee, CMSE, Michigan State University</b> <i>Member</i>	<b>2017-Present</b>
<b>Faculty Advisory Committee, BMB, Michigan State University</b> <i>Ad Hoc Member</i>	<b>2018</b>
<b>Search Committee, Fixed Term Assistant Professor, Mathematics, Michigan State University</b> <i>Member</i>	<b>2018</b>
<b>Computer Committee, BMB, Michigan State University</b> <i>Member</i>	<b>2015-2017</b>
<b>Committee on Undergraduate Minor, CMSE, Michigan State University</b> <i>Member</i>	<b>2015-2017</b>
<b>Tiger Talks, Department of Chemistry, University of Chicago</b> <i>Co-chair, Graphic Designer</i> Ran a series of talks featuring senior graduate students presenting to an audience of their peers.	<b>2009-2010</b>
<b>PSD Social Committee, Physical Sciences Division, University of Chicago</b> <i>Beer Baron</i> Helped organize many social events for graduate students in the PSD, including a weekly happy hour. Responsibilities included sampling and purchasing craft beers from local breweries.	<b>2007-2009</b>
<b>Student Seminar Series, Department of Chemistry, University of Chicago</b> <i>Co-creator, Student Interviewer</i> The goal of this seminar series was to provide junior graduate students with an intimate window into the lives of accomplished academics in chemistry. Two live, one-on-one interviews were conducted with Professors Harry Gray and Fraser Stoddart in front of an audience of graduate students.	<b>2007</b>
<b>Chemistry Students' Union, Department of Chemistry, University of Toronto</b> <i>President</i> Along with a small group of students from my cohort, I transformed the CSU from a defunct organization to a vibrant, active team of students that is still in operation today. The CSU organizes social and academic events for undergraduate students in the Department of Chemistry.	<b>2005-2006</b>
<b>First-year Learning Communities, University of Toronto</b>	



*Student Mentor*

**2005-2006**

Led a weekly course that helped integrate first-year students into undergraduate life. The course was designed to teach academic and personal skills that help students succeed in a University environment. Responsibilities included developing a curriculum, making lesson plans, and leading a class of 24 students.