

C. Keith Cassidy

CONTACT INFORMATION

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RESEARCH INTERESTS

Molecular structure and function of bacterial chemosensory arrays, physical principles of sensory signal transduction in bacterial chemotaxis, applications of high-performance computing and machine learning to biomolecular simulations.

EDUCATION

University of Illinois at Urbana-Champaign, Urbana, IL

Ph.D., Physics, Dec 2016 (Advisor: Prof. Klaus Schulten)

M.S., Physics, May 2013

University of Arkansas, Fayetteville, AR

B.S., Physics, May, 2010 (Advisor: Prof. Gay Stewart)

RESEARCH EXPERIENCE

University of Oxford, Oxford, England

Postdoctoral Researcher.

Fall, 2018 - Present

- Advisors: Prof. Mark Sansom & Dr. Phill Stansfeld, Department of Biochemistry, Structural Bioinformatics and Computational Biochemistry Unit.

University of Illinois at Urbana-Champaign, Urbana, IL

Postdoctoral Researcher.

Spring, 2017 - Fall, 2018

- Advisor: Prof. Zan Luthey-Schulten, Department of Chemistry, Center for the Physics of Living Cells (CPLC).

Research Assistant.

Spring, 2012 - Fall, 2016

- Advisor: Prof. Klaus Schulten, Department of Physics, Theoretical and Computational Biophysics Group (TCBG).
- Dissertation: Molecular Modeling and Simulation of Bacterial Chemosensory Arrays.

University of Arkansas, Fayetteville, AR

Research Assistant.

Fall, 2008 - Spring, 2010

- Advisor: Prof. Jak Tchakalian, Department of Physics, Complex-Oxide Nanomaterials Laboratory.
- Research interests: High-temperature superconductivity in engineered nano-structures.

PUBLICATIONS

- Yang, W., **Cassidy, C. K.**, Ames, P., Diebolder, C., Schulten, K., Luthey-Schulten, Z., Parkinson, J. S., Briegel, A. (2019) In situ conformational changes of the *Escherichia coli* serine chemoreceptor in different signaling states. *mBio*, *In press*.
- **Cassidy, C. K.**, Himes, B. A., Luthey-Schulten, Z., Zhang, P., (2018) CryoEM-based hybrid modeling approaches for structure determination. *Current Opinion in Microbiology*, 43:14-23.
- Stone, J. E., Perilla, J. R., **Cassidy, C. K.**, Schulten, K., (2016) GPU-accelerated molecular dynamics clustering analysis with openACC. *In Parallel Programming with openACC*, Elsevier.
- Goh, B. C., Hadden, J. A., Bernardi, R. C., Singharoy, A., McGreevy, R., Rudack, T., **Cassidy, C. K.**, Schulten, K., (2016) Computational Methodologies for Real-

Space Structural Refinement of Large Macromolecular Complexes. *Annual Review of Biophysics*, 45:253-278.

- **Cassidy, C. K.***, Himes, B. A.*, Alvarez, F. J.*, Ma, J., Zhao, G., Perilla, J. R., Schulten, K., Zhang, P., (2015) CryoEM and Computer Simulations Reveal a Novel Kinase Conformational Switch in Bacterial Chemotaxis Signaling. *eLife*, 10.7554/eLife.08419.
- Perilla, J. R., Goh, B. C., **Cassidy, C. K.**, Liu, B., Bernardi, R. C., Rudack, T., Yu, H., Wu, Z., Schulten, K., (2015) Molecular Dynamics Simulations of Large Macromolecular Complexes. *Current Opinion in Structural Biology*, 31:64-74.
- Fraiberg, M., Afanjar, O., **Cassidy, C. K.**, Gabashvili, A., Schulten, K., Levin, Y., Eisenbach, M., (2014) CheY's Acetylation Sites Responsible for Generating Clockwise Flagellar Rotation in Escherichia coli. *Molecular Microbiology*, 95:231-244.

PUBLICATIONS
(IN PROGRESS)

- **Cassidy, C. K.**, Himes, B. A., Luthey-Schulten, Z., Zhang, P., *Conformational Dynamics of CheA kinase in Escherichia coli Core Chemosensing Complex*.
- Ames, P., **Cassidy, C. K.**, Luthey-Schulten, Z., Parkinson, J. S. *Effects of controllable mutations on transmembrane signaling in E. coli serine receptor*.

FUNDING

Grant: BB/S003339/1 (2018-2021)

Source: Biotechnology and Biological Sciences Research Council

Amount: £1,186,865

Title: Assembly and Dynamics of Bacterial Chemosensory Signaling Arrays

PI: Peijun Zhang

Role: Research Co-Investigator

COMPUTER
ALLOCATIONS

Grant: PSCA17034P (2017-2018)

Machine/Location: Anton 2, Pittsburgh Supercomputing Center

Computer Time: 460,000 MD Units (full allocation)

Title: Transmembrane Signaling in a Canonical Bacterial Chemoreceptor

PI: Zan Luthey-Schulten

Role: Co-PI

RESEARCH
PRESENTATIONS

- **Talk:** *The E. coli Core Signaling Unit: Hybrid Modeling and MD Simulations*. Receptor Fest 21st Annual Meeting. Aug 2018. Cornell University, Ithaca, NY.
- **Poster:** *Molecular Simulations of E. coli Serine Receptor and Sensory Complex*. Gordon Research Conference: Sensory Transduction in Microorganisms. Jan 2018. Ventura Beach, CA.
- **Invited Talk:** *Computing the Bacterial Brain: Molecular Dynamics Simulations of Chemosensory Arrays*. Biochemistry Seminar. Nov 2017. Oxford University, Oxford, England.
- **Invited Talk:** *Computing the Bacterial Brain: Molecular Dynamics Simulations of Chemosensory Arrays*. Biology Seminar. Nov 2017. Leiden University, Leiden, Netherlands.
- **Talk:** *Molecular Dynamics Simulations of E. coli Serine Receptor in Extreme Modification States*. Receptor Fest 20th Annual Meeting. Jul 2017. University of Utah, Salt Lake City, UT.
- **Talk:** *Molecular Modeling and Simulation of Bacterial Chemosensory Arrays on Blue Waters*. Blue Waters Annual Symposium. May 2017. Sunriver, OR.

- **Poster:** *Molecular Modeling and Simulation of the E. coli Serine Receptor*. Bacterial Signaling and Locomotion XIV. Jan 2017. New Orleans, LA.
- **Talk:** *Adventures in Modeling the E. coli Serine Receptor*. Receptor Fest 19th Annual Meeting. Aug 2016. University of California Santa Barbara, Santa Barbara, CA.
- **Invited Talk:** *Structure and Dynamics of Bacterial Chemosensory Arrays*. Gordon Research Conference: Sensory Transduction in Microorganisms. Jan 2016. Ventura Beach, CA.
- **Poster:** *Molecular Insights into the Signaling Mechanism of the Histidine Kinase CheA within an Intact Chemosensory Array*. Gordon Research Seminar: Sensory Transduction in Microorganisms. Jan 2016. Ventura Beach, CA.
- **Talk:** *Modeling the Four-helix Transmembrane Bundle of the E. coli Serine Receptor*. Receptor Fest 18th Annual Meeting. Aug 2015. University of Colorado, Boulder, CO.
- **Invited Talk:** *Structure and Dynamics of Bacterial Chemosensory Arrays*. Medical Microbiology and Immunology Seminar. Jun 2015. University of Wisconsin, Madison, WI.
- **Invited Talk:** *All-atom Structure and Dynamics of an Intact Bacterial Chemosensory Array*. Bacterial Signaling and Locomotion XIII. Jan 2015. Tucson, AZ.
- **Poster:** *Molecular Insights into the Signaling Mechanism of the Histidine Kinase CheA within an Intact Chemosensory Array*. Biophysical Society 59th Annual Meeting. Feb 2015. Baltimore, MD.
- **Talk:** *All-atom Structure and Dynamics of an Intact Bacterial Chemosensory Array*. Receptor Fest 17th Annual Meeting. Jul 2014. University of Utah, Salt Lake City, UT.
- **Talk:** *The Bacterial Brain: All-atom Description of a Chemosensory Array using Blue Waters*. Blue Waters Annual Symposium. May 2014. Urbana, IL.
- **Poster:** *All-atom Structure and Dynamics of an Intact Bacterial Chemosensory Array*. Biophysical Society 58th Annual Meeting. Feb 2014. San Francisco, CA.

TEACHING
EXPERIENCE

Graduate Teaching Assistant.

- PHYS 101 (Fall 2010, Spring 2011) - Ranked “Outstanding TA” by students.
- PHYS 211 (Fall 2011, Spring 2012) - Ranked “Outstanding TA” by students.

Teaching Assistant for TCBG “Hands-on” Workshop on Computational Biophysics

- Berkeley, CA (Fall 2015)
- Pittsburgh, PA (Spring 2015, Spring 2014)
- Urbana, IL (Fall 2017, Spring 2015, Fall 2013)
- Atlanta, GA (Fall 2014)

Teaching Assistant for CPLC Summer School

- Urbana, IL (Summer 2016, 2012, 2011)

Misc.

- Guidance for Physics Students (GPS) Mentor (Fall 2015 - Fall 2016)
- Physics and Calculus tutor (Spring 2012 - Fall 2016)