

Peter M. Kekeneshuskey, Ph.D.

Department of Cell & Molecular Physiology
Loyola University Chicago
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(708) 216-8635

EDUCATION

<i>Doctorate of Philosophy</i> , Chemistry California Institute of Technology, Pasadena, CA	Spring 2009
<i>Bachelor of Science</i> , Chemistry University of North Carolina, Asheville, NC <i>Summa Cum Laude</i>	May 2001

PROFESSIONAL EXPERIENCE

<i>Loyola University Chicago Stritch School of Medicine, Chicago IL</i> Associate Professor, Department of Cell & Molecular Physiology Director of the Cell and Molecular Simulation Resource Center (CaMSiRC)	2019-present
<i>University of Kentucky, Lexington, KY</i> Assistant Professor, Department of Chemistry Adjunct Faculty, Department of Chemical and Materials Engineering	2014 - 2019
<i>University of California San Diego, San Diego CA.</i> [JA McCammon, AD McCulloch] Postdoctoral fellow	2010 - 2014
<i>Arete Associates, Staff Scientist, Northridge CA</i> Staff Scientist	2007 - 2010
<i>Sandia National Laboratory, Albuquerque, NM.</i> [PS Crozier] Summer Internship	summer 2005
<i>California Institute of Technology, Pasadena, CA.</i> [WA Goddard, III] Graduate Student	2001 - 2007
<i>Freie Universitaet zu Berlin, Berlin, Germany.</i> [EW Knapp] Fulbright fellow	2001 - 2002
<i>U. North Carolina, Asheville, NC.</i> [G Heard, BE Holmes] Undergraduate researcher	1999 - 2001
<i>University of Cincinnati, OH.</i> [T Beck, W Connick] Summer researcher	summer 2000

(May 29, 2020)

RESEARCH EMPHASIS

Computational science (physiology, chemistry and biophysics)

- Systems modeling of cardiac and other eukaryotic cells
- Molecular dynamics modeling of regulatory proteins,
- Partial differential equation modeling of small molecule transport
- [Pubmed](#) and [Google Scholar](#)

AWARDS

Faculty

- Nominee for [University of Kentucky \(UK\)](#) Faculty Mentor of the Year 2018
- UK Office of Undergraduate Research's Faculty Mentor of the Week 2018
- Doctoral New Investigator Grant from the American Chemical Society 2017
- UK Arts & Sciences Award for Innovative Teaching 2017
- Recognized as "Teacher who made a difference" (UK) 2016
- UK Nominee for Blavatnik National Awards for Young Scientists 2016-17
- UK Nominee for 2016 Simon's Investigator of Math Modeling of Living Systems award 2015

Post-graduate

- National Institutes of Health Ruth Kirschstein Postdoctoral Fellow 2013
- American Heart Association Western States Affiliates Postdoctoral Fellow 2013
- Vice President Discretionary Award (Arete Associates) 2010

Graduate

- DOE Computational Science Graduate Fellow 2004-2006
- National Science Foundation Fellow (declined for CSGF, 2003) 2002-2003
- Department of Defense Fellowship (declined for NSF) 2001
- Fulbright Fellow (Germany) 2001

Undergraduate

- Manly Wright Award, Valedictorian of Graduating Class 2001
- Outstanding Senior of the Western Carolinas American Chemical Society 2001
- USA Today All-Academic 3rd Team 2001
- Barry Goldwater Scholar in Science and Mathematics 2000-2001
- W. Carolina ACS Schweizerhalle Scholarship 2000-2001
- Phi Eta Sigma National Honors Fraternity 1998
- Albina Mills Academic Scholarship 1998-2001
- 4th Place UNCA Olivia-Jones Freshman Creative Writing Contest 1999

High School

- Eagle Scout 1998
- Lion's Eye Bank Scholarship for Post-Secondary Education 1998
- Presidential Scholar 1998
- National Honors Society 1997

PUBLICATIONS

* equal contribution, ⁺ undergraduate author

Italicized articles are under review

- *E. C. Cook, B. Sun, **P.M. Kekenés-Huskey** and T.P. Creamer, "Electrostatic Forces Mediate Fast Association of Calmodulin and the Intrinsically Disordered Regulatory Domain of Calcineurin." (arXiv: [1611.04080](#))*

(3/40 as Associate Professor at Loyola University Chicago)

1. Rahmaninejad et al 'Co-localization and confinement of ecto-nucleotidases modulate extracellular adenosine nucleotide distributions' (in print, PLOS Comp Bio, 2020)
2. Sun et al, S100A1 Calcium Binding and Post-translational modifications (in print, Frontiers in Molecular Biosciences 2020)
3. Sun, B., Vaughan, D., Tikunova, S., Creamer, T. P., Davis, J. P., **P.M. Kekenés-Huskey**. (2019). Calmodulin-Calcineurin Interaction beyond the Calmodulin-Binding Region Contributes to Calcineurin Activation. Biochemistry 2019, 58, 39, 4070-4085 (PMID [31483613](#))

(13/40 as Assistant Professor at University of Kentucky)

4. Colli, D. F.⁺, Blood, S. R.⁺, Sankarankutty, A. C., Sachse, F. B., Frisk, M., Louch, W. E., **P.M. Kekenés-Huskey**. (2019). A Matched-Filter-Based Algorithm for Subcellular Classification of T-System in Cardiac Tissues. Biophysical Journal, 116(8), 1386-1393. (PMID [30979553](#))
5. Sun, B., Stewart, B. D., Kucharski, A. N.⁺, **P.M. Kekenés-Huskey** (2019). Thermodynamics of Cation Binding to the Sarcoplasmic Reticulum Calcium ATPase Pump and Impacts on Enzyme Function. Journal of Chemical Theory and Computation, 15(4), 2692-2705. (PMID [30807147](#))
6. Shen, X., Brink, J. van den, Hou, Y., Colli, D., Le, C., Kolstad, T. R., **P.M. Kekenés-Huskey**, Louch, W. E. (2019). 3D dSTORM imaging reveals novel detail of ryanodine receptor localization in rat cardiac myocytes. The Journal of Physiology, 597(2), 399-418. (PMID [30412283](#)) (top 10% most downloaded papers)
7. Wagh, P., Zhang, X., Blood, R.⁺, **P.M. Kekenés-Huskey**, Rajapaksha, P., Wei, Y., Escobar, I. C. (2019). Increasing Salt Rejection of Polybenzimidazole Nanofiltration Membranes via the Addition of Immobilized and Aligned Aquaporins. Processes, 7(2), 76. (PMID [31179235](#))
8. Sun, B., Cook, E. C., Creamer, T. P., and **P.M. Kekenés-Huskey** (2018). Electrostatic control of calcineurin's intrinsically-disordered regulatory domain binding to calmodulin. Biochimica et Biophysica Acta (BBA) - General Subjects, 1862(12), 2651-2659. (PMID [30071273](#))
9. B Chun, BD Stewart, DD Vaughan⁺ AS Bachstetter, **P.M. Kekenés-Huskey**, (2019). Simulation of P2X-mediated calcium signalling in microglia. The Journal of Physiology, 597(3), 799-818. (PMID [30462840](#))
10. B Sun, R Blood⁺ S Atalay, D Colli⁺ SE Rankin, BL Knutson and **P.M. Kekenés-Huskey**, "Simulation-based characterization of electrolyte and small molecule diffusion in imaged oriented mesoporous silica thin films", (chemRxiv: [5533066](#)) (in press)
11. Stewart, B. D., Scott, C. E., McCoy, T. P., Yin, G., Despa, F., Despa, S., and **P.M. Kekenés-Huskey**. (2018). "Computational modeling of amylin-induced calcium dysregulation in rat ventricular cardiomyocytes." Cell Calcium, 71, 65-74. (PMID [29604965](#))
12. JK Siddiqui, SB Tikunova, SD Walton, M Meyer, PP de Tombe, N Neilson, **P.M. Kekenés-Huskey**, HE Salhi, PML Janssen, BJ Biesiadecki, JP Davis, "Myofilament Calcium Sensitivity: Consequences of the Effective Concentration of Troponin I," Frontiers in Physiology, 2016, 7:632. (PMID [28066265](#))

13. A.N. Kucharski⁺, C.E. Scott, J.P. Davis and **P.M. Keken-Huskey**, "Understanding Ion Binding Affinity and Selectivity in β Parvalbumin Using Molecular Dynamics and Mean Sphere Approximation Theory," J Phys Chem B, 2016, 120(33):8617-30 (PMID [28066265](#))
14. **P.M. Keken-Huskey**, C. E. Scott, and S. Atalay, "Quantifying the influence of the crowded cytoplasm on ionic diffusion," J Phys Chem B 2016, 120(33):8696-706 (PMID [27327486](#))
15. C. E. Scott and **P.M. Keken-Huskey**, "Molecular basis of calcium-induced structural changes of human S100A1," Biophys J, Mar. 2016, 110(5):1052-1063 (PMID [26958883](#))
16. **P.M. Keken-Huskey**, C. Eun, and A. McCammon, "Enzyme localization, crowding, and buffers collectively modulate diffusion-influenced signal transduction: Insights from continuum diffusion modeling," Journal of Chemical Physics, 2015, 143(9):1-12. (PMID [26342355](#))

(25/40 up through postdoctoral studies)

17. S. Lindert, Y. Cheng, **P.M. Keken-Huskey**, M. Regnier, and J. A. McCammon, "Effects of HCM cTnI mutation R145G on troponin structure and modulation by PKA phosphorylation elucidated by molecular dynamics simulations.," Biophys J, vol. 108, no. 2, pp. 395-407, Jan. 2015. (PMID [25606687](#))
18. N. Wang, S. Zhou, **P.M. Keken-Huskey**, B. Li, and J. A. McCammon, "Poisson-Boltzmann vs. Size-modified Poisson-Boltzmann Electrostatics Applied to Lipid Bilayers," J Phys Chem B, p. 141126142529007, Nov. 2014. (PMID [25426875](#))
19. V. T. Metzger, C. Eun, **P.M. Keken-Huskey**, G. Huber, and J. A. McCammon, "Electrostatic Channeling in P. falciparum DHFR-TS: Brownian Dynamics and Smoluchowski Modeling," Biophys J, vol. 107, no. 10, pp. 2394-2402, Nov. 2014. (PMID [25418308](#))
20. Y. Cheng, S. Lindert, **P.M. Keken-Huskey**, V. S. Rao, R. J. Solaro, P. R. Rosevear, R. Amaro, A. D. McCulloch, J. A. McCammon, and M. Regnier, "Computational Studies of the Effect of the S23D/S24D Troponin I Mutation on Cardiac Troponin Structural Dynamics," Biophys J, vol. 107, no. 7, pp. 1675-1685, Oct. 2014.(PMID [25296321](#))
21. **P.M. Keken-Huskey**, A. K. Gillette, and J. A. McCammon, "Predicting the influence of long-range molecular interactions on macroscopic-scale diffusion by homogenization of the Smoluchowski equation," The Journal of chemical physics, vol. 140, no. 17, p. 174106, May 2014.(PMID [23293662](#))
22. J. Hake, **P.M. Keken-Huskey**, and A. D. McCulloch, "Computational modeling of subcellular transport and signaling," Current Opinion in Structural Biology, vol. 25, pp. 92-97, Apr. 2014.(PMID [24509246](#))
23. C. Eun, **P.M. Keken-Huskey***, V. T. Metzger, and J. A. McCammon, "A model study of sequential enzyme reactions and electrostatic channeling.," Journal of Chemical Physics, vol. 140, no. 10, pp. 105101-105101, Mar. 2014.(PMID [24628210](#))
24. **P.M. Keken-Huskey**, T. Liao, A. K. Gillette, J. E. Hake, Y. Zhang, A. P. Michailova, A. D. McCulloch, and J. A. McCammon, "Molecular and subcellular-scale modeling of nucleotide diffusion in the cardiac myofilament lattice.," Biophys J, vol. 105, no. 9, pp. 2130-2140, Nov. 2013.(PMID [24209858](#))
25. T. Liao, Y. Zhang, **P.M. Keken-Huskey**, Y. Cheng, A. Michailova, A. D. McCulloch, M. Holst, and J. McCammon, "Multi-core CPU or GPU-accelerated Multiscale Modeling for Biomolecular Complexes," Molecular Based , pp. 164-179, Oct. 2013.(PMID [24352481](#))
26. C. Eun, **P.M. Keken-Huskey**, and J. A. McCammon, "Influence of neighboring reactive particles on diffusion-limited reactions.," Journal of Chemical Physics, vol. 139, no. 4, pp. 044117-044117, Jul. 2013.(PMID [23901970](#))
27. P. Setny, R. Baron, **P.M. Keken-Huskey**, J. A. McCammon, and J. Dzubiella, "Solvent fluctuations in hydrophobic cavity-ligand binding kinetics," Proc Natl Acad Sci USA, vol. 110,

- no. 4, pp. 1197-1202, Jan. 2013.(PMID [23297241](#))
28. **P.M. Kekenés-Huskey**, S. Lindert, and J. McCammon, "Molecular basis of calcium-sensitizing and desensitizing mutations of the human cardiac troponin C regulatory domain: a multi-scale simulation study.," PLOS Computational Biology, vol. 8, no. 11, pp. e1002777-e1002777, Nov. 2012.(PMID [23209387](#))
 29. **P.M. Kekenés-Huskey***, V. Metzger*, B. Grant, and J. McCammon, "Calcium binding and allosteric signaling mechanisms for the sarcoplasmic reticulum Ca(2+) ATPase.," Protein Sci., vol. 21, no. 10, pp. 1429-1443, Oct. 2012.(PMID [22821874](#))
 30. J. Hake, A. G. Edwards, Z. Yu, **P.M. Kekenés-Huskey**, A. P. Michailova, J. A. McCammon, M. J. Holst, M. Hoshijima, and A. D. McCulloch, "Modelling cardiac calcium sparks in a three-dimensional reconstruction of a calcium release unit.," The Journal of Physiology, vol. 590, no. 18, pp. 4403-4422, Sep. 2012.(PMID [22495592](#))
 31. S. Lindert, **P.M. Kekenés-Huskey**, G. Huber, L. Pierce, and J. McCammon, "Dynamics and calcium association to the N-terminal regulatory domain of human cardiac troponin C: a multiscale computational study.," J Phys Chem B, vol. 116, no. 29, pp. 8449-8459, Jul. 2012.(PMID [22329450](#))
 32. **P.M. Kekenés-Huskey**, Y. Cheng, J. Hake, F. Sachse, J. Bridge, M. Holst, A. McCulloch, J. McCammon, and A. Michailova, "Modeling effects of L-type ca(2+) current and na(+)-ca(2+) exchanger on ca(2+) trigger flux in rabbit myocytes with realistic T-tubule geometries.," Front Physiol, vol. 3, pp. 351-351, Jan. 2012.(PMID [23060801](#))
 33. Y. Cheng, **P.M. Kekenés-Huskey**, J. E. Hake, M. J. Holst, J. A. McCammon, and A. P. Michailova, "Multi-scale continuum modeling of biological processes: from molecular electrodiffusion to sub-cellular signaling transduction," Comput Sci Discov, vol. 5, no. 1, p. 015002, 2012.(PMID [23505398](#))
 34. **P.M. Kekenés-Huskey**, A. Gillette, J. Hake, and J. A. McCammon, "Finite-element estimation of protein-ligand association rates with post-encounter effects: applications to calcium binding in troponin C and SERCA," Comput Sci Discov, vol. 5, no. 1, p. 014015, 2012.(PMID [23293662](#))
 35. S. Lindert, **P.M. Kekenés-Huskey**, and J. A. McCammon, "Long-Timescale Molecular Dynamics Simulations Elucidate the Dynamics and Kinetics of Exposure of the Hydrophobic Patch in Troponin C," Biophys J, vol. 103, no. 8, pp. 1784-1789, 2012. (PMID [23083722](#))
 36. **P.M. Kekenés-Huskey**, A Monte Carlo-based torsion construction algorithm for ligand design. Doctoral Thesis, 2009.
 37. J. Heo, S. Han, N. Vaidehi, J. Wendel, **P.M. Kekenés-Huskey**, and W. Goddard III, "Prediction of the 3D Structure of FMRF-amide Neuropeptides Bound to the Mouse MrgC11 GPCR and Experimental Validation," ChemBioChem, vol. 8, no. 13, pp. 1527-1539, 2007.(PMID [17647204](#))
 38. J. D. Ferguson, N. L. Johnson, **P.M. Kekenés-Huskey**, W. C. Everett, G. L. Heard, D. W. Setser, and B. E. Holmes, "Unimolecular Rate Constants for HX or DX Elimination (X = F, Cl) from Chemically Activated CF 3CH 2CH 2Cl, C 2H 5CH 2Cl, and C 2D 5CH 2Cl: Threshold Energies for HF and HCl Elimination," J. Phys. Chem. A, vol. 109, no. 20, pp. 4540-4551, May 2005.(PMID [16833790](#))
 39. A. E. Cho, J. A. Wendel, N. Vaidehi, **P.M. Kekenés-Huskey**, W. B. Floriano, P. K. Maiti, and W. A. Goddard, "The MPSim-Dock hierarchical docking algorithm: Application to the eight trypsin inhibitor cocrystals," J Comput Chem, vol. 26, no. 1, pp. 48-71, 2004.(PMID [15529328](#))
 40. **P.M. Kekenés-Huskey**, I. Muegge, and M. Rauch, "A molecular docking study of estrogenically active compounds with 1, 2-diarylethane and 1, 2-diarylethene pharmacophores," Bioorganic& medicinal, 2004.(PMID [15556769](#))

41. **P.M. Kekenesh-Huskey**, N. Vaidehi, W. B. Floriano, and W. Goddard III, "Fidelity of phenylalanyl-tRNA synthetase in binding the natural amino acids," J Phys Chem B, vol. 107, no. 41, pp. 11549-11557, 2003.

FUNDING

†principal investigator °co-principal investigator *co-investigator +significant contributions

Active

1 R35 GM124977 (Kekenes-Huskey)† 09/01/17-08/31/22
NIH/NIGMS \$1,558,386.00 (incl. indirect)
"Probing cellular intracellular calcium signaling and sensing through computation"
The major goals of this project is to develop multi-scale tools to predict intracellular calcium signaling, from single molecules to the cell.

1 R35 GM124977 S1 (Kekenes-Huskey)† Supplemental award. 09/01/19-08/31/20
NIH/NIGMS \$249,422
"Computational characterization of microglial P2X signaling and phenotypes in Alzheimer's patients
The major goals of this project to do automate the characterization of microglial phenotypes in AD tissue based on microscopy and RNA sequence data.

Petroleum Research Fund (Kekenes-Huskey)† 01/01/18-08/01/20 (0.25 calendar month)
American Chemical Society \$110,000 (incl. indirects)
"Multi-Scale Modeling of Methane Permeation in Defect-Containing Zeolitic Materials"
Major goals include developing multi-physical, multi-scale models of gaseous substrates in highly-structured, zeolitic materials.

Completed

Igniting Research Collaborations Award ° 07/19
University of Kentucky \$25,000
"Molecular Dynamic Simulations Improve the Clinical Value of Genetic Testing"
PKH declined

NASA EPSCoR (Brehm, Kekenes-Huskey)° 05/01/19-12/31/19 (0.25 calendar month)
NASA \$40,000 (incl. indirects)
"Development of a RANS-Based Wall-Model for Cartesian Grid Navier-Stokes Solvers"
Major goals include developing multi-physical, multi-scale models of fluid flow.

5 U01 HL133359 02 (Campbell)+ 08/03/2018-07/31/22
NIH/NIGMS (\$610,274)
'Multiscale modeling of inherited cardiomyopathies and therapeutic interventions'
The major goal of this project is to create multi-scale models of cardiac function and myopathies, from the molecular to whole-organ levels. **PKH provides molecular simulation expertise but does not currently draw funds from this award.**

4 P20 GM103527 09 (Cassis)* 09/01/17-08/31/20, (1.67 calendar months)
NIH/NIGMS \$2,257,498
Pilot Support through "Center of Biomedical Research Excellence (COBRE) on Obesity and Cardiovascular Diseases (COCVD)
The major goal of this project is to enhance the competitiveness of junior faculty with research programs. **PKH lab was supported through a 50K pilot award.**

1 R56 HL131782 01 (Satin)* 09/16-08/17, (< 1 calendar month)
NIH/NHLBI \$524,989 (incl. indirect)
"Monomeric G-protein and cardioprotection from heart failure"
The major goal of this project is to model excitation/contraction coupling domain in a transverse

tubule dyadic junction.

University of Kentucky, Igniting Research Collaborations Award † 05/15-08/15
"Simulations of dysregulated intracellular Ca²⁺-handling in diabetic cardiomyopathy"
PKH: \$25,495 / Total: \$25,495.

University of Kentucky Startup † 07/01/14-06/30/17
PKH: \$240,000/ Total: \$240,000 (2.0 calendar month)

NIGMS, Competitive Renewal (3 P41GM103426-20)⁺ 2014
Total: \$1,990,191

NHLBI, National Research Service Award† 2013
PKH: \$84,000/ Total \$84,000

American Heart Association, Western Affiliates Postdoctoral Fellowship† 2013
PKH: \$88,000 / Total: \$88,000

NIGMS, Supplementary Award (3 P41 GM103426-19S1)⁺ 2012
Total: \$367,613

DoD/Navy, Phase I SBIR ⁺ 2010
"Image Fusion for Submarine Imaging Systems"
Total:\$99991

DoD, Phase I SBIR ⁺ 2010
"Investigation of the Debye Effect for Submarine Detection"
Total: \$79,995

DoD, Phase II SBIR⁺ 2009
Algorithm for Submarine Periscope Systems
Total: \$1,267,015

TEACHING EXPERIENCE

- Function of the Human Body (FHB) Small Group Sessions, LUC, Chicago, IL 2020
- UNIV 102: Introduction to Computation and Modeling of physiological systems, LUC, Chicago, IL 2020
- CHE 580: Introduction to computation and modeling of chemical systems, UK, Lexington, KY 2018-
- "Introduction to multi-scale modeling", Jilin University, Changchun, China 2017
- CHE 446G: Physical Chemistry for Engineers, UK, Lexington, KY 2016-
- "Mathematics of Physical Chemistry Boot Camp", UK, Lexington KY 2015-
- CHE 441: Physical Chemistry Lab, UK, Lexington, KY 2015,17
- CHE 105: Gen College Chemistry I, UK, Lexington, KY 2014-15
- CHEM 280: Applied Bioinformatics, Guest Lecturer, UCSD, San Diego, CA 2013
- BENG/CHEM 276: Numerical Analysis for Multi-Scale Biology, Guest Lecturer, UCSD, San Diego, CA 2013
- Mesoscale Modeling, NBCR Summer Institute, UCSD, San Diego, CA 2012
- "Sub-cellular models of calcium diffusion", NBCR Summer Institute, UCSD, San Diego, CA 2011
- "Multi-scale Modeling of Cardiac Function", Workshop at International Conference on Biological Physics, San Diego, CA 2011
- "Continuum Diffusion in Molecular Systems, NBCR Summer Institute, UCSD, San Diego, CA 2011
- "Special Topics in Signal Processing", Co-lecturer at Arete Associates staff education workshop series, Northridge, CA 2008

SERVICE

Loyola University Chicago

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|---|-------|
| Centralized Admissions Committee | 2019- |
| Director of the Cell and Molecular Simulation Resource Center (CaMSiRC) | 2019- |
| Chair's Advisory Council | 2019- |

University of Kentucky

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|---|----------------------|
| Center of Computational Sciences Faculty Advisory Committee | 2015-2019 |
| Research/Scholarship Advisory Committee | 2014-2019 |
| Naff 2016 Symposium Organizer | 2015-2016 |
| Graduate Recruiting Committee | 2014-2017 |
| Seminar Committee | 2017-2018 |
| Website Committee | 2014-2015, 2018-2019 |
| Faculty Advisor to Society of Postdocs | 2014-2016 |

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|--|--------------|
| Sarah Flury (Physiol), Thesis Committee | 2020 |
| Simon Schmitt (ME), Thesis Committee | 2019 |
| Azin Akbari (CME), Outside Examiner | 2018 |
| Chamikara Karunasena (Che), Thesis Committee | 2018-present |
| Surya Aryal (Che), Thesis Committee | 2018-present |
| Japheth Gado (Chem E), Thesis Committee | 2018-present |
| Danielle Schaper (Phys), Thesis Committee | 2017-present |
| Angela Collier (Phys), Thesis Committee | 2017-present |
| Lakshya Malhotra (Phys), Thesis Committee | 2017-present |
| Amira Yu (Chem E), Thesis Committee | 2017 |

Brandon Franklin (Bio), Thesis Committee	2017
Wang Hua (Mech E), Thesis Committee	2017
Joseph Duke (Chem), Thesis Committee	2016-present
Xiaolu Zhang (Chem), Thesis Committee	2015

After Hours Residence Life Outreach	2016
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External

REAL (Read, Excel, Achieve, Lead) Program, Maxwell Elementary	2019
CREST High School Outreach program	2016-present

Computation Science Graduate Fellowship Selection Committee	2019
National Science Centre - proposal review	2018
NSF Review Panel	2016 (2), 2018 (2), 2019 (1)
Quarterly XRAC Review Committee	2015-present
Computation Science Graduate Fellowship Screening Committee	2012-present
Petroleum Research Fund proposal review	2015, 2018

Manuscripts reviewed

J Mol Cell Card, International J of Med Sci, Neural Computing and Applications, PLOS Comp. Bio., Comp. and Struct. Biotech., EBJO	2020
PLOS Comp. Bio., PLOS One, Neural Computing and Applications (2), Proteins, Molecules, Journal of Biomolecular Structure & Dynamics, Applied Mathematical Letters, Front. Mol. Biosci., Scientific Reports	2019
Journal of Computer Aided Molecular Design, Journal of Physical Chemistry, Computers in Biology and Medicine, Archives of Biochemistry and Biophysics	2018
PLOS One, Scientific Reports, Journal of Cheminformatics, Biochemistry (2), European Biophysics Journal, eLife, Mathematical Biosciences, Biophysical Journal, Journal of Chemical Physics, Biochemistry (2), Journal of Chemical Physics (3), PLOS One	2017
European Biophysics Journal, Journal of Physical Chemistry B, Biophysical Journal	2016
Journal of Chemical Physics, Biophysical Journal (3), FEBS Letters	2015
PNAS	2014
	2013

Miscellaneous

Cardiovascular Research Day Poster Judge, MACE Symposium Poster Judge	2018
Handling editor for Frontiers Special Topic Issue	2015
Coordinator of Caltech Alumni Association events in San Diego/Lexington	2012-present
Mini-symposium co-organizer at SIAM Life Sciences meeting, San Diego, CA	2012
Chaired session at Domain Decomposition Meeting, San Diego, CA	2011
JAM Steering committee	2011-2014

TRAINING

Center of Research in Obesity and Cardiovascular Disease Monthly Meeting	2017-2018
Presentation U! Faculty Fellow, Lexington, KY	2016
College of Arts and Sciences Teaching Workshop, Lexington, KY	2016
Cottrell Scholars New Faculty Workshop, Washington DC	2015
Center for the Physics of Living Cells Summer School (UIUC)	2013
Scientific Ethics (UCSD)	2013

College Classroom (Center for Teaching Development, UCSD)	2013
San Diego Lab Management Symposium participant	2010

ADVISING

Postdoctoral scholars

• Caitlin E Scott, Ph.D. Assistant Professor, Hendrix College Biophysical Society Travel Award	2014-16
• Selcuk Atalay, Ph.D.	2015-16
• Ben Chun, Ph.D.	2017-present
• Kalyan Immadisetty, Ph.D.	2019-
• Bin Sun, Ph.D.	2020-
• Xuan Fang, Ph.D.	2020-

Graduate students

• Bin Sun (CHE), Ph.D. Dec 2019 University of Kentucky Graduate Fellowship Research Challenge Trust Fund Outstanding Performance on the Oral Qualifying Exam	2015-2019 2016 2017-2018 2017
• Darin Vaughan (CHE)	2018-2019
• Hadi Rahmani (PHY)	2018-2020
• Tom Pace (PHY) Huffaker Travel Award	2017- 2019
• Charles Adeniran (CHE) Lyman T Johnson Fellow	2017-2018 2018
• Brad Stewart (CHE) Graduate Teaching award	2015-2017 2017

Undergraduate students

• Amir Kucharski (CHE) Gaines Fellowship Admission to WUSTL MD/Ph.D. program	2014-7
• Ryan Blood (CME) Admission to Notre Dame graduate school Notebaert Fellow	2016-2018 2018 2018
• Andrew Mondragon (CME)	2017
• Dylan Colli (CME) Second place in Graduate Poster Competition AiCHE American Heart Association USTiCR fellow	2016-2019 2017 2018
• Angela Hinchie (CHE) Admission to University of Pittsburgh graduate school	2016
• Darin Vaughan (MA,CHE) Admission to University of Kentucky graduate school	2017-2018
• Rachel Boone (CME) National Science Foundation Graduate Research Fellow	2017-2019

High school

- Mikhail Essa
- Shashank Bhatta (Dunbar High School)

2019-
2017-2019

PRODUCTS

SMOLFIN Diffusion-limited association reactions

ENZYMEKINETICSACS Spatially-decoupled biochemical reactions

SMOLHOMOG Homogenized Smoluchowski solver

HOMOGENIZATION Multi-scale estimates of diffusion tensors

SARCOMERE Metabolism in half-sarcomere

Additional software is available at bitbucket.org/huskeypm and bitbucket.org/pkhlabs/pkh-lab-analyses/

MEMBERSHIPS

American Chemical Society

Biophysical Society

American Heart Association

INVITED TALKS

2020

Illinois Institute of Technology, Chicago, IL *Invited talks deferred due to Coronavirus Pandemic*

2019

University of South Florida, Tampa, FL; University of California Riverside, CA; University of Virginia, Charlottesville, VA; California State University Los Angeles, CA; City of Hope, Duarte, CA, Illinois Institute of Technology, Chicago, IL; Loyola University Chicago (Lakeshore), Chicago, IL;

2018

Myofilament Meeting, Madison, WI, University of Kentucky (Department of Biomedical Engineering), Lexington KY, University of Kentucky (Department of Physiology), Lexington KY Commonwealth Computational Summit, Lexington, KY Carnegie Mellon/University of Pittsburgh, Pittsburgh, PA, University of West Virginia, Morgantown, WV

2017

Earlham College, Richmond IN, Berea College, Berea, KY, Vanderbilt University, Nashville, TN

2016

Illinois Institute of Technology, Chicago, IL, Rush University, Chicago, IL, University of Kentucky (Departments of Math, Physics), Lexington, KY, University of Missouri, Columbia, MO, Truman State University, Kirksville, MO, Tennessee Technical University, Cookeville, TN Myofilament Meeting 2016, Madison, WI, California Institute of Technology, Pasadena, CA, University of California San Diego, San Diego, CA

2015

Indiana State University, Terre Haute, IN, Simula Summer School, Norway, Oslo, Bluegrass Molecular Biophysics Symposium, Lexington, KY, Salt Lake City, UT

2014

University of Kentucky Dept. of Chemical Engineering, Lexington, KY, Furman University, Greenville, SC, Oak Ridge National Labs, Oak Ridge, TN, Invited Poster at SciMix SERMACs meeting, Nashville, TN, American Chemical Society National Meeting, Dallas, CA, University of Arizona, Tucson, AZ, Loyola University Health Sciences Campus, Chicago, IL,

2013

Northeastern University, Boston, MA, University of Washington, Seattle, WA, University of North Carolina, Asheville, NC, Fall National ACS meeting, Indianapolis, IN, Simula Research Laboratory, Norway, Oslo, CVRTI, University of Utah, Salt Lake City, UT, Department of Chemistry, University of Utah, Salt Lake City, UT

2011

Gordon Research Seminar on Calcium Signaling, Waterville, ME, Mathematics and Biochemistry-Biophysics Seminar at UCSD, San Diego, CA

PRESENTATIONS

Muscle Forum, University of Kentucky	2015
Society of Post-docs, University of Kentucky	2015
Biophysical Society Annual Meeting	2015
Heart Working Group, University of Kentucky	2014
Students of the American Chemical Society, University of Kentucky	2014
"Multi-scale simulations of diffusion-influenced reactions", Poster at Gordon Research Conference, Mount Snow Resort, NH	2014
"Multi-scale simulations of diffusion-influenced reactions", Talk at William Goddard, III's Birthday Symposium, Pasadena, CA	2014
"Multi-scale simulations of diffusion-influenced reactions", Poster at ACS National Meeting, Dallas, TX	2014
"Multi-scale Continuum Modeling and Simulation of Cardiac Function, Talk at Nifty Fifty, Kearny High School, San Diego, CA	2014
"A Markov-state model for the regulation of the sarcoplasmic reticulum Ca^{2+} ATPase by phospholamban", Poster at Biophysical Society Meeting, San Francisco, CA	2014
"Continuum diffusion: a language for bridging molecular and cellular scale signaling", Talk at Georgia State University, Atlanta, GA	2013
"Building a molecular to cellular-scale understanding of Troponin function through simulation", Talk at Ohio State University, Columbus, OH	2013
"Continuum diffusion: a language for bridging molecular and cellular scale signaling", Talk at Carnegie Mellon, Pittsburgh, PA	2013
"Modeling Calcium Dynamics in Realistic Rabbit Ventricular Myocytes with Several Transverse Tubules", Poster at Alternative Muscle Club Meeting, University of California, San Diego	2013
"Multi-scale Continuum Modeling and Simulation of Cardiac Function, Talk at Nifty Fifty, Sweet-	

water High School, El Cajon, CA	2013
"Substrate association as a two stage process: the diffusional encounter and post-encounter binding", Talk at Modeling Diffusional Encounter and Subsequent Events Mini-Symposium, San Diego, CA	2012
"Multi t-tubule modeling: M-times better than a single t-tubule", Talk at Cardiac Physiome Brain- storming session, San Diego, CA	2012
"Molecular and sub-cellular modeling of cardiac Troponin C calcium handling", Talk at SIAM Life Sciences Meeting, San Diego, CA	2012
"Molecular electrostatics and Diffusion", Talk at NBCR Summer Institute, San Diego, CA	2012
"High-level science: a dogma for research and employment?", Talk at CSGF Alumni Meeting, Wash- ington DC	2012
"Modeling Calcium Dynamics in Realistic Rabbit Ventricular Myocytes with Several Transverse Tubules", Poster at Gordon Conference on Muscle Excitation Contraction, Les Diableret, Switzer- land	2012
"Stochastic gating regulates calcium association rates in Troponin C and SERCA", Talk at American Chemical Society Meeting, San Diego, CA	2012
"Molecular and sub-cellular modeling of Ca ²⁺ signaling in cardiomyocytes", Talk for Nifty Fifty, San Diego High School, San Diego, CA	2012
"Modeling Calcium Dynamics in Realistic Rabbit Ventricular Myocytes with Several Transverse Tubules", Poster at Biophysical Society Meeting, San Diego, CA	2012
"Contributions of structural t-tubule heterogeneities in local Ca ²⁺ signaling in rabbit ventricular myocytes", Poster at NBCR Summer Institute, UCSD, San Diego, CA (Awarded Best Poster)	2011
"Contributions of structural t-tubule heterogeneities in local Ca ²⁺ signaling in rabbit ventricular myocytes", Poster at Cardiac Physiome Workshop, Oxford, England	2011
"Contributions of structural t-tubule heterogeneities in local Ca ²⁺ signaling in rabbit ventricular myocytes", Poster at Gordon Conference on Calcium Signaling, Waterville, ME	2011
"Accelerated molecular dynamics of sarcoplasmic reticulum Ca ²⁺ ATPase (SERCA) structural tran- sitions", Poster at International Conference on Biological Physics, San Diego, CA	2011

"Sub-cellular Ca^{2+} signaling in cardiac myocytes", Talk at NBCR RAC meeting, UCSD, San Diego, CA 2011

"Contributions of structural t-tubule heterogeneities and membrane Ca^{2+} flux localization to local Ca^{2+} signaling in rabbit ventricular myocytes", Poster at Biophysical Society Meeting, Baltimore, MD 2011

"Multi-scale Continuum Modeling and Simulation of Cardiac Function", Talk at Nifty Fifty High School Outreach, Carlsbad, CA 2011

"Effects of membrane calcium flux localizations and realistic t-tubule geometry on cardiac excitation contraction coupling", Mini-talk at Biological Diffusion and Brownian Dynamics Brainstorm 2 at UCSD, San Diego, CA 2010