Peter M. Kekenes-Huskey, Ph.D.

(February 8, 2019)

Department of Chemistry
Graduate Faculty in the
Department of Chemical and Materials Engineering
University of Kentucky
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EDUCATION

Doctorate of Philosophy, Chemistry
California Institute of Technology, Pasadena, CA — Spring 2009

Bachelor of Science, Chemistry
University of North Carolina, Asheville, NC — May 2001
Summa Cum Laude

PROFESSIONAL EXPERIENCE

University of Kentucky, Lexington, KY — 2014 - present
Assistant Professor of Chemistry
Adjunct Faculty in Chemical and Materials Engineering

University of California San Diego, San Diego CA[JA McCammon, AD McCulloch] — 2010 - 2014
Postdoctoral fellow

Arete Associates, Staff Scientist, Northridge CA — 2007 - 2010
Staff Scientist

Sandia National Laboratory, Albuquerque, NM. [PS Crozier] — summer 2005
Summer Internship

California Institute of Technology, Pasadena, CA. [WA Goddard, III] — 2001 - 2007
Graduate Student

Freie Universitaet zu Berlin, Berlin, Germany. [EW Knapp] — 2001 - 2002
Fulbright fellow

U. North Carolina, Asheville, NC. [G Heard, BE Holmes] — 1999 - 2001
Undergraduate researcher

University of Cincinnati, OH. [T Beck, W Connick] — summer 2000
Summer researcher

RESEARCH EMPHASIS

Computational chemistry and biophysics

- Systems modeling of calcium signaling in cardiac and other eukaryotic cells
- Molecular dynamics modeling of regulatory proteins, finite element 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*

(12/37 as faculty member)

1. Sun, B, Stewart, B, Kucharski^{+}, A, **P.M. Kekenes-Huskey**, 'Cation binding to SERCA' (bioarxiv 507996, accepted J Chem Theory Comp)
2. Shen, X., Brink, J. van den, Hou, Y., Colli, D., Le, C., Kolstad, T. R., **P.M. Kekenes-Huskey**, Louch, W. E. (2018). 3D dSTORM imaging reveals novel detail of ryanodine receptor localization in rat cardiac myocytes. The Journal of Physiology. (in print, (PMID 30412283))
3. P. Wagh, X. Zhang, R. Blood^{+}, **P.M. Kekenes-Huskey**, P. Rajapaksha, Y. Wei and I. Escobar, 'Alignment and Immobilization of Aquaporins on Polybenzimidazole Nanofiltration Membranes' (accepted)
4. *Dylan Colli^{+} et al,* **P.M. Kekenes-Huskey**, *"GPU accelerated detection and classication of myocyte transverse tubule ultra-structure", (bioarxiv 371328, under revison)*
5. Sun, B., Cook, E. C., Creamer, T. P., and **P.M. Kekenes-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)
6. Byeongjae Chun, Bradley D Stewart, Darin D Vaughan^{+} Adam S Bachstetter, **P.M. Kekenes-Huskey**, "Simulation of P2X-mediated calcium signaling in microglia", The Journal of Physiology, (in print, (PMID 30462840))
7. Bin Sun, Ryan Blood^{+} Selcuk Atalay, Dylan Colli^{+} Stephen E. Rankin, Barbara L. Knutson and **P.M. Kekenes-Huskey**, "Simulation-based characterization of electrolyte and small molecule diffusion in imaged oriented mesoporous silica thin films", (chemRxiv: 5533066) (in press)
8. Stewart, B. D., Scott, C. E., McCoy, T. P., Yin, G., Despa, F., Despa, S., and **P.M. Kekenes-Huskey**. (2018). "Computational modeling of amylin-induced calcium dysregulation in rat ventricular cardiomyocytes." Cell Calcium, 71, 65-74. (PMID 29604965)
9. *E. C. Cook, B. Sun,* **P.M. Kekenes-Huskey** *and T.P. Creamer,"Electrostatic Forces Mediate Fast Association of Calmodulin and the Intrinsically Disordered Regulatory Domain of Calcineurin." 2016. (arXiv: 1611.04080) (under revision)*
10. JK Siddiqui, SB Tikunova, SD Walton, M Meyer, PP de Tombe, N Neilson, **P.M. Kekenes-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)
11. A.N. Kucharski^{+}, C.E. Scott, J.P. Davis and **P.M. Kekenes-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)
12. **P.M. Kekenes-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)
13. C. E. Scott and **P.M. Kekenes-Huskey**, "Molecular basis of calcium-induced structural changes of human S100A1," Biophys J, Mar. 2016, 110(5):1052-1063 (PMID 26958883)
14. **P.M. Kekenes-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)

(25/37 up through postdoctoral studies)

15. S. Lindert, Y. Cheng, **P.M. Kekenes-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)

16. N. Wang, S. Zhou, **P.M. Kekenes-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)
17. V. T. Metzger, C. Eun, **P.M. Kekenes-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)
18. Y. Cheng, S. Lindert, **P.M. Kekenes-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)
19. **P.M. Kekenes-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)
20. J. Hake, **P.M. Kekenes-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)
21. C. Eun, **P.M. Kekenes-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)
22. **P.M. Kekenes-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)
23. T. Liao, Y. Zhang, **P.M. Kekenes-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)
24. C. Eun, **P.M. Kekenes-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)
25. P. Setny, R. Baron, **P.M. Kekenes-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)
26. **P.M. Kekenes-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)
27. **P.M. Kekenes-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)
28. J. Hake, A. G. Edwards, Z. Yu, **P.M. Kekenes-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)
29. S. Lindert, **P.M. Kekenes-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)

30. **P.M. Kekenes-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)
31. Y. Cheng, **P.M. Kekenes-Huskey**, J. E. Hake, M. J. Holst, J. A. McCammon, and A. P. Michailova, "Multi-scale continuum modeling of biological processes: from molecular electro-diffusion to sub-cellular signaling transduction," Comput Sci Discov, vol. 5, no. 1, p. 015002, 2012.(PMID 23505398)
32. **P.M. Kekenes-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)
33. S. Lindert, **P.M. Kekenes-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)
34. **P.M. Kekenes-Huskey**, A Monte Carlo-based torsion construction algorithm for ligand design. Doctoral Thesis, 2009.
35. J. Heo, S. Han, N. Vaidehi, J. Wendel, **P.M. Kekenes-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)
36. J. D. Ferguson, N. L. Johnson, **P.M. Kekenes-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)
37. A. E. Cho, J. A. Wendel, N. Vaidehi, **P.M. Kekenes-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)
38. **P.M. Kekenes-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)
39. **P.M. Kekenes-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 (2.00 calendar month)
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.

Petroleum Research Fund (Kekenes-Huskey)† 01/01/18-12/31/19 (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.

NASA EPSCoR (Brehm, Kekenes-Huskey)° xx/01/19-xx/31/20 (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.**

Completed

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

- 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

University of Kentucky

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

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

After Hours Residence Life Outreach	2016

External

REAL (Read, Excel, Achieve, Lead) Program, Maxwell Elementary	2019

CREST High School Outreach program 2016-present

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

Manuscripts reviewed

Molecules, Journal of Biomolecular Structure & Dynamics, Applied Mathematical Letters 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, 2017
Biochemistry (2), Journal of Chemical Physics (3), PLOS One 2016
European Biophysics Journal, Journal of Physical Chemistry B, Biophysical Journal 2015
Journal of Chemical Physics, Biophysical Journal (3), FEBS Letters 2014
PNAS 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-present
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. 2014-16
  Assistant Professor, Hendrix College
  Biophysical Society Travel Award
- Selcuk Atalay, Ph.D. 2015-16
- Ben Chun, Ph.D. 2017-present
- Kalyan Immadisetty, Ph.D. 2019-

Graduate students

- Charles Adeniran (CHE) 2017-2018
  Lyman T Johnson Fellow 2018

- Tom Pace (PHY) 2017-
  Huffaker Travel Award 2019

- Brad Stewart (CHE) 2015-2017
  Graduate Teaching award 2017

- Bin Sun (CHE) 2015-
  University of Kentucky Graduate Fellowship 2016
  Research Challenge Trust Fund 2017-2018
  Outstanding Performance on the Oral Qualifying Exam 2017

Undergraduate students

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

High school

- Shashank Bhatta (Dunbar High School) 2017-

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/pkhlab/pkh-lab-analyses/

MEMBERSHIPS

American Chemical Society
Biophysical Society
American Heart Association

INVITED TALKS

2019

University of South Florida (Feb), University of California Riverside (Apr), University of Virginia (Apr)

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, Cookesville, 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 Ca2+ 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 Brainstorming 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, Washington DC 2012

"Modeling Calcium Dynamics in Realistic Rabbit Ventricular Myocytes with Several Transverse Tubules", Poster at Gordon Conference on Muscle Excitation Contraction, Les Diableret, Switzerland 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 Ca2+ 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 Ca2+ 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 Ca2+ signaling in rabbit ventricular myocytes", Poster at Cardiac Physiome Workshop, Oxford, England 2011

"Contributions of structural t-tubule heterogeneities in local Ca2+ signaling in rabbit ventricular myocytes", Poster at Gordon Conference on Calcium Signaling, Waterville, ME 2011

"Accelerated molecular dynamics of sarcoplasmic reticulum Ca2+ ATPase (SERCA) structural transitions", Poster at International Conference on Biological Physics, San Diego, CA 2011

"Sub-cellular Ca2+ signaling in cardiac myocytes", Talk at NBCR RAC meeting, UCSD, San Diego, CA 2011

"Contributions of structural t-tubule heterogeneities and membrane Ca2+ flux localization to local Ca2+ 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