Peter M. Kekenes-Huskey, Ph.D.

Department of Cell & Molecular Physiology
Loyola University Chicago, Chicago, IL 60153

pkekeneshuskey@luc.edu
https://pkhlab.sites.luc.edu/

SPECIALIZATIONS

Computational science (physiology, chemistry and biophysics)

- Systems modeling of cardiac and other Eukaryotic cells
- Molecular dynamics modeling of regulatory proteins,
- Partial differential equation-based analyses of small molecule transport
- Computer vision and machine learning

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

Loyola University Chicago Stritch School of Medicine, Chicago IL — 2019-present
Associate Professor, Department of Cell & Molecular Physiology
Director of the Cell and Molecular Simulation Resource Center (CaMSiRC)

University of Kentucky, Lexington, KY — 2014 - 2019
Assistant Professor, Department of Chemistry
Adjunct Faculty, Department of 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

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*

(15/52 as Associate Professor at Loyola University Chicago)

1. Tally et al Monitoring of Inflammation Using an Engineered Biosensor Mouse Model Reveals Tissue- and Sex-specific Responses to Western Diet (accepted)
2. Seflova, J., Habibi, N. R., Yap, J. Q., Cleary, S. R., Fang, X., **P.M. Kekenes-Huskey**, Espinoza-Fonseca, L. M., Bossuyt, J. B., & Robia, S. L. (2022). Fluorescence Lifetime Imaging Microscopy Reveals Sodium Pump Dimers in Live Cells. The Journal of Biological Chemistry, 101865. (PMID 35339486)
3. Immadisetty, K., Alenciks, J.$^{+}$, & **P.M. Kekenes-Huskey**(2022). Modulation of P2X4 pore closure by magnesium, potassium, and ATP. Biophysical Journal. (PMID 35248546)
4. Rahmaninejad, H., Pace, T., Chun, B. J., & **P.M. Kekenes-Huskey**(2022). Crowding within synaptic junctions influences the degradation of nucleotides by CD39 and CD73 ectonucleotidases. Biophysical Journal, 121(2), 309âĂŞ318. (PMID 34922916)
5. Pace, T., Rahmaninejad, H., Sun, B., & **P.M. Kekenes-Huskey** (2021). Homogenization of Continuum-Scale Transport Properties from Molecular Dynamics Simulations: An Application to Aqueous-Phase Methane Diffusion in Silicate Channels. The Journal of Physical Chemistry. B. (PMID 34618464)
6. Sun, B., Fang, X., Johnson, C. N., Hauck, G., Kou, Y., Davis, J. P., and **P.M. Kekenes-Huskey** (2021). Non-Canonical Interaction between Calmodulin and Calcineurin Contributes to the Differential Regulation of Plant-Derived Calmodulins on Calcineurin. Journal of Chemical Information and Modeling. (PMID 34615359)
7. Immadisetty, K., Sun, B., and **P.M. Kekenes-Huskey**(2021). Structural determinants of calcium binding beyond the EF-hand binding site: A study of alpha parvalbumins, J. Phys. Chem. B, 125, 24, 6390-6405 (PMID 34115511)
8. Sun, B., and **P.M. Kekenes-Huskey** (2021). Assessing the Role of Calmodulin's Linker Flexibility in Target Binding. International Journal of Molecular Sciences, 22(9), 4990. (PMID 34066691)
9. Marques, M. A., Landim-Vieira, M., Moraes, A. H., Sun, B., Johnston, J. R., Dieseldorff Jones, K. M., Cino, E. A., Parvatiyar, M. S., Valera, I. C., Silva, J. L., Galkin, V. E., Chase, P. B., **P.M. Kekenes-Huskey**, de Oliveira, G. A. P., and Pinto, J. R. (2021). Anomalous structural dynamics of minimally frustrated residues in cardiac troponin C triggers hypertrophic cardiomyopathy. Chemical Science. (PMID 34163821)
10. van de Locht M, Donkervoort S, de Winter JM, Conijn S, Begthel L, Kusters B, Mohassel P, Hu Y, Medne L, Quinn C, Moore SA, Foley AR, Seo G, Hwee DT, Malik FI, Irving T, Ma W, Granzier H, Kamsteeg EJ, Immadisetty K, **P.M. Kekenes-Huskey**, Pinto JR, Voermans N, Bonnemann CG, Ottenheijm CA.,'Pathogenic variants in TNNC2 cause congenital myopathy due to an impaired force response to calcium', 2021 J Clin Invest. Mar 23:145700. (PMID 33755597)
11. Sun, B., Blood, R^{+}, Atalay, S., Colli, D^{+}, Rankin, S. E., Knutson, B. L., and **P.M. Kekenes-Huskey**(2021). Simulation-based characterization of electrolytes and small molecule diffusion in oriented mesoporous silica thin films. In S. S., M. R., D. T., & C. G.H. (Eds.), Springer Series in Materials Science (Vol. 284, pp. 521-558). Springer, Cham. (link)
12. Ono, M., Burgess, D. E., Schroder, E. A., Elayi, C. S., Anderson, C. L., January, C. T., Sun, B., Immadisetty, K., **P.M. Kekenes-Huskey**, and Delisle, B. P. (2020). Long QT Syndrome Type 2: Emerging Strategies for Correcting Class 2 KCNH2 (hERG) Mutations and Identifying New Patients. Biomolecules, 10(8), 1144. (PMID 32759882)

13. Rahmaninejad, H., Pace, T., Bhatt, S., Sun, B., and **P.M. Kekenes-Huskey** (2020). Co-localization and confinement of ecto-nucleotidases modulate extracellular adenosine nucleotide distributions. PLoS Computational Biology, 16(6), e1007903. (PMID 32584811)

14. Sun, B., and **P.M. Kekenes-Huskey** (2020). Molecular Basis of S100A1 Activation and Target Regulation Within Physiological Cytosolic Ca2+ Levels. Frontiers in Molecular Biosciences, 7. (PMID 32656226)

15. Sun, B., Vaughan, D.$^+$, Tikunova, S., Creamer, T. P., Davis, J. P., **P.M. Kekenes-Huskey**. (2019). Calmodulin-Calcineurin Interaction beyond the Calmodulin-Binding Region Contributes to Calcineurin Activation. Biochemistry 2019, 58, 39, 4070-4085 (PMID 31483613)

(12/52 as Assistant Professor at University of Kentucky)

16. Colli, D. F.$^+$, Blood, S. R.$^+$, Sankarankutty, A. C., Sachse, F. B., Frisk, M., Louch, W. E., **P.M. Kekenes-Huskey**. (2019). A Matched-Filter-Based Algorithm for Subcellular Classification of T-System in Cardiac Tissues. Biophysical Journal, 116(8), 1386-1393. (PMID 30979553)

17. Sun, B., Stewart, B. D., Kucharski, A. N.$^+$, **P.M. Kekenes-Huskey**(2019). Thermodynamics of Cation Binding to the Sarcoendoplasmic Reticulum Calcium ATPase Pump and Impacts on Enzyme Function. Journal of Chemical Theory and Computation, 15(4), 2692-2705. (PMID 30807147)

18. Shen, X., Brink, J. van den, Hou, Y., Colli, D., Le, C., Kolstad, T. R., **P.M. Kekenes-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)

19. Wagh, P., Zhang, X., Blood, R.$^+$, **P.M. Kekenes-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)

20. B Chun, BD Stewart, DD Vaughan$^+$ AS Bachstetter, **P.M. Kekenes-Huskey**, (2019). Simulation of P2X-mediated calcium signalling in microglia. The Journal of Physiology, 597(3), 799-818. (PMID 30462840)

21. 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)

22. 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)

23. 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)

24. 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 27267153)

25. **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)

26. 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)

27. **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)

28. 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)
29. 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)
30. 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)
31. 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)
32. **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)
33. 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)
34. 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)
35. **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)
36. 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)
37. 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)
38. 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)
39. **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)
40. **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)
41. 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)

42. 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)

43. **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)

44. 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)

45. **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)

46. 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)

47. **P.M. Kekenes-Huskey**, A Monte Carlo-based torsion construction algorithm for ligand design. Doctoral Thesis, 2009. (link)

48. 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)

49. 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)

50. 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 co-crystals," J Comput Chem, vol. 26, no. 1, pp. 48-71, 2004.(PMID 15529328)

51. **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)

52. **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.

Pre-print articles (not peer-reviewed)

- *Chun et al, Purinoreceptors and ectonucleotidases control ATP-induced calcium waveforms and calcium-dependent responses in microglia. bioarxiv (under review)*
- *Cleary et al, Inhibitory and Stimulatory Micropeptides Preferentially Bind to Different Conformations of the Cardiac Calcium Pump. bioarxiv (under review)*

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.

20IPA35320141 (Kekenes-Huskey)† 01/01/21-12/31/22
American Heart Association $200,000
"Toward early diagnosis of long QT syndrome using machine learning and molecular dynamics simulation of KCNH2"
This project uses simulation to predict if missense mutations in the KCNH2 gene will cause cardiac disease
*0.58% percentile

Pediatric Cancer Research Trust Fund (Kolesar) * 07/01/20-06/30/22 (0.5 mo)
Kentucky Cabinet for Health and Family Services $629,000
'Macrophage Derived Engineered Vesicles for Preventing Metastasis in Pediatric Osteosarcoma.'
The major goal is to develop a computational approach to predict inflammatory phenotypes in macrophages.

1 R01 xxxx (Robia)* 03/01/22-xxxx (0.60 calendar month)
NIH/NHLBI $ (incl. indirect)
""
Studies of the Na-K ATPase

Completed

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.

58719-DNI6 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.

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

- UNIV 102: Intro. to Physiological systems, LUC, Chicago, IL 2021
- Physiological Methods (Lecture), LUC, Chicago, IL 2020
- Function of the Human Body (FHB) Small Group Sessions, LUC, Chicago, IL 2020-
- UNIV 102: Intro. to Comp. and Modeling of physiological systems, LUC, Chicago, IL 2020
- CHE 580: Intro. 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 2016-2018
- "Mathematics of Physical Chemistry Boot Camp", UK, Lexington KY 2015-2019
- 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, 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

Centralized Admissions Committee 2019-
Director of the Cell and Molecular Simulation Resource Center (CaMSiRC) 2019-
Chair's Advisory Council 2019-
Master of Science Medical Physiology advisor 2020-2021
Faculty Search Committee 2020-
Sarah Flury (Physiol), Thesis Committee 2020-
Sean Cleary (Physiol), Thesis Committee 2020-

University of Kentucky

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

Simon Schmitt (ME), Thesis Committee 2019
Azin Akbari (CME), Outside Examiner 2018
Chamikara Karunasena (Che), Thesis Committee 2018-2019
Surya Aryal (Che), Thesis Committee 2018-2019
Japheth Gado (Chem E), Thesis Committee 2018-2019
Danielle Schaper (Phys), Thesis Committee 2017-2019

Angela Collier (Phys), Thesis Committee	2017-2019
Lakshya Malhotra (Phys), Thesis Committee	2017-2019
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

External

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

Computation Science Graduate Fellowship Selection Committee	2019
National Science Centre - proposal review	2018
NSF Review Panel	2016 (2), 2018 (2), 2019 (1), 2020 (1)
Quarterly XRAC Review Committee	2015-present
Computation Science Graduate Fellowship Screening Committee	2012-present
Petroleum Research Fund proposal review	2015, 2018, 2020-22

Manuscripts reviewed

Biochemistry Frontiers In Molecular Neuroscience, Philosophical Transactions B	2022
Circulation: Genomic and Precision Medicine, Biophysical Journal, PLOS Comp Bio (3), ACS Medicinal Chemistry, Frontiers in Molecular Biosciences, Journal of Physical Chemistry B, STAR protocols	2021
Pfluegers Archiv - European Journal of Physiology, ACS Omega, Circulation: Genomic and Precision Medicine, J Mol Cell Card (3), 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,	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

Editor for International Journal of Molecular Sciences Special Issue	2021
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. 2014-16
  Assistant Professor, Hendrix College
  Biophysical Society Travel Award
- Selcuk Atalay, Ph.D. 2015-16
- Ben Chun, Ph.D. 2017-2021
- Kalyan Immadisetty, Ph.D. 2019-2022
- Bin Sun, Ph.D. 2020-21
  Assistant Professor, Harbin University
- Xuan Fang, Ph.D. 2020-

Masters students

- Geraldine San Ramon
- Peter Varughese

Graduate students

- Bin Sun (CHE), Ph.D. Dec 2019 2015-2019
  Thesis: Multi-Scale Computational Studies of Calcium (Ca2+) Signaling
  University of Kentucky Graduate Fellowship 2016
  Research Challenge Trust Fund 2017-2018
  Outstanding Performance on the Oral Qualifying Exam 2017
- Darin Vaughan (CHE) 2018-2019
- Hadi Rahmani (PHY) 2018-2020
- Tom Pace (PHY) Ph.D. Apr 2021 2017-21
  Thesis: Predicting Material Properties: Applications of Multi-Scale Multiphysics Numerical Modeling to Transport Problems in Biochemical Systems and Chemical Process Engineering
  Huffaker Travel Award 2019
- Charles Adeniran (CHE) 2017-2018
  Lyman T Johnson Fellow 2018
- Brad Stewart (CHE) 2015-2017
  Graduate Teaching award 2017

Undergraduate students

- Rohan Sethi 2021-
- Karthik Myneni 2021-
- David Ilc 2020-
- Mohammed Muqsith 2020-
- Joshua Bruno 2020-
- Michael Muzupappa 2020-
- Jeremiah Jacob-Dolan (CHE) 2020-2021
  Admission to Boston University Graduate School
- Amir Kucharski (CHE) 2014-7
  Gaines Fellowship
  Admission to WUSTL MD/Ph.D. program
- Ryan Blood (CME) 2016-2018
  Admission to Notre Dame graduate school 2018
  Notebaert Fellow 2018
- Andrew Mondragon (CME) 2017
- Dylan Colli (CME) 2016-2019
  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) 2017-2018
  Admission to University of Kentucky graduate school
- Rachel Boone (CME) 2017-2019
  National Science Foundation Graduate Research Fellow
  Admission to Vanderbilt Graduate Program

High school

- Mikhail Essa (Lagrange High School) 2019-2020
- Shashank Bhatta (Dunbar High School) 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/pkhlab/pkh-lab-analyses/

MEMBERSHIPS

American Chemical Society
Biophysical Society

American Heart Association

INVITED TALKS

2022

Loyola University Chicago (Biology Seminar), Chicago, IL; American Chemical Society, San Diego, CA

2021

Loyola University Chicago (Bioinformatics Program), Chicago, IL;

2020

University of North Carolina, Asheville, NC; Illinois Institute of Technology, Chicago, IL; Loyola University Chicago (Integrated Cellular Biology Program), Chicago, IL; Wayne State University, Detroit, MI

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, 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

Training Outcomes

How many years have you been training students.
Since 2014 as a faculty member.

How many undergraduates you have trained.
14 Undergrads, 2 High School students 16 total of which there were 2 women.

Important outcomes/accomplishments of these students (papers, abstracts, presentations, current positions).

- *High school student outcomes:* Both students are now in college (University of Kentucky and Cornell University).
- *Undergraduate student outcomes:* Nearly all of the undergraduates that have worked in my lab and since graduated enrolled in Ph.D. or MD/Ph.D. programs. These students attend WUSTL (MD/Ph.D), Notre Dame, Vanderbilt, Pittsburgh and Boston, among others. One student joined my lab as a graduate student. Seven of my lab's publications feature contributions from undergraduate or high school school authors (oftentimes with multiple undergraduate authors), including two first-author publications. Several of these students have received undergraduate scholarships, of which two have received graduate fellowships, including an award from the National Science Foundation.

Training Opportunities
Background Our lab uses computational and experimental approaches to uncover how biophysical properties of molecules and proteins shape cardiac and immune function at a cellular level. Our extramural funding in this area has supported applications relevant to chronic pain, Alzheimer's disease, anti-tumor therapeutics and cardiac arrhythmias that could usher in new treatment strategies. These applications include investigations of cellular pathways controlled by calcium-dependent proteins such as troponin C (muscle contraction), calmodulin (calcium 'sensing'), parvalbumin (calcium 'buffering') and purinergic receptors (ATP-dependent calcium channels).

Nature of Work: Our lab's expertise sits at the interface of Chemistry, Physiology and Biophysics. We use and develop a variety of computational approaches for investigating biology systems, including molecular simulations, statistical physics, computer vision and numerical algorithms. In complement, our lab measures enzyme kinetics and performs live and fixed cell microscopy experiments to inform or validate our computational approaches. Undergraduates participate in all aspects of our work. We are highly collaborative, as we work closely with several laboratories at Loyola and institutions world-wide that specialize in cardiac and neurological function. Our team comprises multi-disciplinary scientists at many career stages, from high school students to postdoctoral scholars, which provides for an excellent learning environment.

Lab Training Plan: My lab currently comprises several senior postdocs that spearhead specific research topics, such as protein function, systems biology and biomolecule mass transport. New students are initially assigned to work with a postdoc aligned with their interests, so that they can become familiarized with a given research topic and the necessary scientific background. In the first few weeks, I usually meet with the new student individually to help streamline their transition into my lab. As part of this process, I give students tutorial assignments germane to their interests that introduce them to the computational techniques. Within weeks, the students segue into research-level problems, for which they can make their own unique scientific contributions. Additionally, my lab is loosely organized into subgroups that generally have a postdoc and one or more junior lab members to facilitate training and discovery. I meet with these subgroups weekly to discuss progress and challenges; while I encourage all members to participate, contributions are generally expected to be informal. We also have a standing group (biweekly) and joint group (monthly) meetings where formal presentations are given and constructively critiqued. Our department also offers weekly journal clubs and seminars during the academic year, which all lab members are encouraged to attend. I maintain a physical and virtual open door policy to enable impromptu conversations with all lab members; I use a group-wide live messaging system (Slack) to support a virtual environment

in which trainees can easily reach me or fellow group members for help and feedback. As applicable and often required by the university, lab members take safety orientations and responsible conduct of research classes. We practice open science to encourage data exchange and reproducibility.

Research Project Environment Our lab is funded with an R35 award from the National Institute of General Medical Sciences and an Innovative Project Award from the American Heart Association. Our dry lab includes several high performance workstations and a ten-node, GPU-enabled computational cluster for simulations. Our wet lab includes sufficient consumables and equipment to conduct our experimental work; we work closely with our departmental colleagues to utilize shared equipment including microscopes, cell culturing setups, and plate readers. Our department organizes activities for undergraduate researchers and provides some level of stipend support beyond the PI's funds.