**Kim F. Wong**

**(a) Professional Preparation**

Reed College, Portland, OR, USA Chemistry/Physics B.A. 1996

University of Texas, Austin, TX, USA Chemistry Ph.D. 2001

**(b) Appointments**

**University of Pittsburgh**, Dept. of Chemistry and Center for Simulation and Modeling, **Research Assistant Professor** (Oct 2008– )

University of Utah, Dept. of Chemistry, Postdoctoral Fellow (Aug 2004–Oct 2008 )

The Pennsylvania State University, Dept. of Chemistry, Postdoctoral Fellow (Aug 2001–Aug 2004 )

**(c) Contributions to Code Development Projects**

1. **WESTPA** (Weighted Ensemble Simulation Toolkit with Parallelization and Analysis), Lillian Chong, University of Pittsburgh. WESTPA is an open-source software package that provides a high-performance computing framework for carrying out extended-timescale simulations of rare events with rigorous kinetics using the weighted ensemble algorithm.
2. **RHEA** (Regional Healthcare Ecosystem Analyst), Bruce Lee, University of Pittsburgh. RHEA is a software package for simulating the impact of intervention measures on disease outbreaks within a realistic model of a healthcare system.

**(d) Grants in Support of Research**

CDC NCEZID IPA Contract: 14IPA1408987. 05/16/2014 – 09/30/2014

**(e) Publications**

1. M. C. Zwier, J. L. Adelman, J. W. Kaus, A. J. Pratt, **K. F. Wong**, N. B. Rego, E. Suarez, S. Lettieri, D. W. Wang, M. Grabe, D. M. Zuckerman, L. T. Chong, “WESTPA: An Interoperable, Highly Scalable Software Package for Weighted Ensemble Simulation and Analysis,” J. Chem. Theory Comput., **11**, 800-809 (2015).
2. S. M. Bartsch, S. S. Huang, **K. F. Wong**, T. R. Avery, B. Y. Lee, “The Spread and Control of Norovirus Outbreaks Among Hospitals in a Region: A Simulation Model,” Open Forum Infect. Dis., **1**, ofu030, 1-7 (2014).
3. A. Maries, N. Mays, M. O. Hunt, **K.F. Wong**, W. Layton, R. Boudreau, C. Rosano, G. E. Marai, “GRACE: A visual comparison framework for integrated spatial and non-spatial geriatric data,” IEEE Trans. Vis. Comput. Graph., **19**, 2916-2925 (2013).
4. B. Y. Lee, S. L. Yilmaz, **K. F. Wong**, S. M. Bartsch, S. Eubank, Y. Song, T. R. Avery, R. Christie, S. T. Brown, J. M. Epstein, J. I. Parker, S. S. Huang, “Modeling the regional spread and control of vancomycin-resistant enterococci,” Am. J. Infect. Control, **41**, 668-673 (2013).
5. B. Y. Lee, **K. F. Wong**, S. M. Bartsch, S. L. Yilmaz, T. R. Avery, S. T. Brown, Y. Song, A. Singh, D. S. Kim and S. S. Huang. “The Regional Healthcare Ecosystem Analyst (RHEA): a simulation modeling tool to assist infectious disease control in a health system.” J. Am. Med. Inform. Assoc., **20**, e139-e146 (2013).
6. B. Y. Lee, S. M. Bartsch, **K. F. Wong**, A. Singh, T. R. Avery, D. S. Kim, S. T. Brown, C. R. Murphy, S. L. Yilmaz, M. A. Potter, and S. S. Huang. “The Importance of Nursing Homes in the Spread of Methicillin-resistant Staphylococcus aureus (MRSA) Among Hospitals,” Medical Care, **51**, 205-215 (2013).
7. B. Y. Lee, A. Singh, S. M. Bartsch, **K. F. Wong**, D. S. Kim, T. R. Avery, S. T. Brown, C. R. Murphy, S. L. Yilmaz, and S. S. Huang. “The Potential Regional Impact of Contact Precaution Use in Nursing Homes to Control Methicillin-Resistant *Staphylococcus aureus*,” Infection Control and Hospital Epidemiology, **34**, 151-160 (2013).
8. B. Y. Lee, S. M. Bartsch, **K. F. Wong**, S. L. Yilmaz, T. R. Avery, A. Singh, Y. Song, D. S. Kim, S. T. Brown, M. A. Potter, R. Platt, and S. S. Huang. “Simulation Shows Hospitals that Cooperate on Infection Control Obtain Better Results than Hospitals Acting Alone,” Health Affairs, 31, 2295-2303 (2012).
9. B. Y. Lee, Y. Song, S. M. Bartsch, D. S. Kim, A. Singh, T. R. Avery, S. T. Brown, S. L. Yilmaz, **K. F. Wong**, M. A. Potter, D. S. Burke, R. Platt, and S. S. Huang.  “Long-Term Care Facilities: Important Participants of the Acute Care Facility Social Network?,” PLoS ONE, **6**, e29342 (2011).
10. B. Y. Lee, S. M. McGlone, **K. F. Wong**, S. L. Yilmaz, T. R. Avery, Y. Song, R. Christie, S. Eubank, S. T. Brown, J. M. Epstein, J. I. Parker, D. S. Burke, R. Platt, and S. S. Huang. “Modeling the spread of methicillin-resistant Staphylococcus aureus (MRSA) outbreaks throughout the hospitals in Orange County, California,” Infection Control and Hospital Epidemiology, **32**, 562-72 (2011).
11. **K. F. Wong**, J. L. Sonnenberg, F. Paesani, T. Yamamoto, J. Vaníček, W. Zhang, H. B. Schlegel, D. A. Case, T. E. Cheatham III, W. H. Miller, and G. A. Voth, “Proton Transfer Studied Using a Combined Ab Initio Reactive Potential Energy Surface with Quantum Path Integral Methodology,” J. Chem. Theory Comput., **6**, 2566-2580 (2010).
12. J. L. Sonnenberg, **K. F. Wong**, G. A. Voth, and H. B. Schlegel, “Distributed Gaussian Valence Bond Surface Derived from Ab Initio Calculations,” J. Chem. Theory Comput., **5**, 949-961 (2009).
13. J. B. Watney, A. V. Soudackov, **K. F. Wong,** and S. Hammes-Schiffer, “Calculation of the transition state theory rate constant for a general reaction coordinate: Application to hydride transfer in an enzyme,” *Chem. Phys. Lett.*, **418**, 268-271 (2006).
14. A. Sergi, J. B. Watney, **K. F. Wong**, and S. Hammes-Schiffer, "Freezing a single distal motion in dihydrofolate reductase," *J. Phys. Chem. B,* **110**, 2435-2441 (2006).
15. C. M. Maupin, **K. F. Wong**, A. V. Soudackov, S. Kim, and G. A. Voth, “A Multistate Empirical Valence Bond Description of Protonatable Amino Acids,” *J. Phys. Chem. A,* **110**, 631-639 (2006).
16. **K. F. Wong**, T. Selzer, S. J. Benkovic, and S. Hammes-Schiffer, “Impact of distal mutations on the network of coupled motions correlated to hydride transfer in dihydrofolate reductase," *Proc. Nat. Acad. Sci. USA,* **102***,* 6807-6812 (2005)*.*
17. **K. F. Wong**, J. B. Watney, and S. Hammes-Schiffer, "Analysis of electrostatics and correlated motions for hydride transfer in dihydrofolate reductase," *J. Phys. Chem. B,* **108**, 12231-12241 (2004).
18. **K. F. Wong**, B. Bagchi, and P. J. Rossky, “Distance and Orientation Dependence of Excitation Transfer Rates in Conjugated Systems: Beyond the Förster Theory,” *J. Phys. Chem. A*, **108**, 5752-5763 (2004).
19. **K. F. Wong** and P. J. Rossky, “Solvent-Induced Electronic Decoherence: Configuration Dependent Dissipative Evolution for Solvated Electron Systems,” *J. Chem. Phys*., **116**, 8429-8438 (2002).
20. **K. F. Wong** and P. J. Rossky, “Dissipative Mixed Quantum-Classical Simulation of the Aqueous Solvated Electron System,” *J. Chem. Phys*., **116**, 8418-8428 (2002).
21. **K. F. Wong**, M. S. Skaf, C.-Y. Yang, P. J. Rossky, B. Bagchi, D. Hu, J. Yu, and P. F. Barbara, “Structural and Electronic Characterization of Chemical and Conformational Defects in Conjugated Polymers,” *J. Phys. Chem. B*, **105**, 6103-6107 (2001).
22. **K. F. Wong** and P. J. Rossky, “Mean-Field Molecular Dynamics with Surface Hopping: Application to the Aqueous Solvated Electron,” *J. Phys. Chem. A*, **105**, 2546-2556 (2001).
23. C.-Y. Yang, **K. F. Wong**, M. S. Skaf, and P. J. Rossky, “Instantaneous Normal Mode Analysis of Hydrated Electron Solvation Dynamics,” *J. Chem. Phys*., **114**, 3598-3611 (2001).
24. D. Hu, J. Yu, **K. F. Wong**, B. Bagchi, P. J. Rossky, and P. F. Barbara, “Collapse of Stiff Conjugated Polymers with Chemical Defects into Ordered, Cylindrical Conformations,” *Nature*, **405**, 1030-1033 (2000).

**(f) Poster and Oral Presentations**

1. **K. F. Wong**, “Risk of HPC Investment vs Return on HPC Investment.” Lightning Talks. CASC Spring Meeting. March 31-April 2, 2015. Arlington, VA.
2. **K. F. Wong**, S. L. Yilmaz, R. A. Christie, S. M. McGlone, S. S. Huang, and B. Y. Lee. “Agent-Based Modeling of the Spread of Methicillin-Resistant Staphylococcus aureus (MRSA) Outbreaks within a Hospital Network.” Poster presentation at SC11. November 12-18, 2011; Seattle, WA.
3. S. L. Yilmaz, **K. F. Wong**, R. A. Christie, S. M. McGlone, Y. Song, S. T. Brown, A. Singh, R. Bailey, T. R. Avery, S. Eubank, J. M. Epstein, J. I. Parker, D. S. Burke, R. Platt, D. S. Kim, S. S. Huang, B. Y. Lee, “Modeling and Investigation of Disease Outbreaks in Hospital Networks with an Agent Based Model,” TeraGrid Conference: Extreme Digital Discovery, Salt Lake City, Utah, Poster presentation, Jul. 18--21, (2011).
4. S. M. McGlone, S. S. Huang, **K. F. Wong**, S. L. Yilmaz, Y. Song, T. R. Avery, R. A. Christie, S. T. Brown, J. Epstein, S. Eubank, D. S. Burke, R. Platt, B. Y. Lee. “Modeling the Spread of Methicillin-Resistant Staphylococcus aureus Throughout Orange County, California.” The Society for Healthcare Epidemiology of America (SHEA) Annual Scientific Meeting. April 1-4, 2011; Dallas, TX.
5. **K. F. Wong**. “The Approximate Pursuit of Rigorous Science.” Poster presentation at the Epistemology of Modeling and Simulation National Conference. April 1-3, 2011; Pittsburgh, PA.
6. **K. F. Wong**, S. L. Yilmaz, R. A. Christie, B. Y. Lee, and S. S. Huang. “Agent-Based Model of Patient Flow within a Hospital Network: Understanding How Changes in One Hospital can Affect Other Hospitals in a Region.” Poster presentation at SC10. November 13-19, 2010; New Orleans, LA.
7. S. M. McGlone, S. S. Huang, **K. F. Wong**, S. L. Yilmaz, Y. Song, T. R. Avery, R. Christie, S. T. Brown, S. Eubank, J. M. Epstein, J. I. Parker, D. S. Burke, R. Platt, B. Y. Lee. “An agent-based network model of the spread of Staphylococcus aureus throughout Orange County, California.”  Oral presentation at the Modeling for Public Health Action: From Epidemiology to Operations conference. December 9-10, 2010; Atlanta, GA.

**(g) Synergistic Activities**

1. Mentoring two students within the First Experiences in Research program. Project topic: designing, coding, and modeling the spread of diseases within a UPMC hospital. Spring 2015.
2. XSEDE Campus Champion (2013 - )
3. Reviewer for American Journal of Public Health (2014).
4. Reviewer for The Journal of Physical Chemistry (2014).
5. Training Workshop: “MPI-X Hybrid Programming.” February 23, 25, 27, 2015.
6. Training Workshop: “The Hows and Whats of Using the SaM High Performance Computing Cluster.” January 14, 2015.
7. Physical Chemistry judge for Chem. Dept. Undergraduate Laboratory Poster Session. December 5, 2014.
8. Presentation to the Engineering Graduate Student Organization Coffee Hour. “SaM: Here to Computationally Enable your Graduate Training.” October 3, 2014.
9. Guest Lecturer for BioSc1540: Computational Biology. “Learning High Performance Computing to Accelerate Your Undergraduate Education.” September 29, 2014.
10. Training Workshop: “Special Howto Topics: Accessing Environments for Code Development and Package Building.” September 26, 2014.
11. Training Workshop: “Fundamentals for Effective Usage of the High Performance Computing Cluster.” September 22, 2014.
12. Presentation to the Economics Department. “High-Performance Computing Resources for Enabling Computational Economics.” August 25, 2014.
13. Presentation to Public Health. “Introduction to Using the SaM HPC Cluster for Modeling Public Health Dynamics.” August 8, 2014.
14. Presentation to the Engineering Graduate Student Organization Coffee Hour. “How SaM can Accelerate your Graduate Career.” March 31, 2014.
15. Co-Lecturer. Training Workshop on “Basics of Using the High Performance Computing Cluster at the University of Pittsburgh” and “Advanced Usage of the High Performance Computing Cluster.” February 25-26, 2014.
16. Guest Lecturer for ME2223/MSE2113: Nanoscale Modeling and Simulations: Density Functional Theory. “Leveraging High Performance Computing for Nanoscale Modeling and Simulations.” January 27, 2014.
17. Guest Lecturer for CHE3935: Particle-based Materials Modeling. “Using High Performance Computing for Particle-based Materials Modeling.” January 15, 2014.
18. Presentation to Swanson School of Engineering Lunch and Learn. “SaM I Am: How the Center for Simulation and Modeling can Increase the Quality and Impact of your Computationally-Enabled Research.” January 9, 2014.
19. Guest Lecturer for BioSc1540: Computational Biology. “Using High Performance Computing to Accelerate Research at the University.” October 4, 2013.
20. Organized booth marketing SaM at Science 2013: Convergence. October 2-4, 2013.
21. Guest Lecturer for ME2107: High Performance Computing Algorithms and Methods. “Scientific Software Development on the University of Pittsburgh HPC Cluster.” September 10, 2013.
22. Co-Lecturer. Training Workshop on “Introduction to the HPC Resources at the University of Pittsburgh” and “Advanced Topics on Effective Usage of the High Performance Computing Cluster.” July 18-19, 2013.
23. Co-Lecturer: Workshop on Introduction to Parallel Programming with OpenMP. University of Pittsburgh, December 13-14, 2012.
24. Co-Lecturer: Workshop on Effective Usage of the High Performance Computing Resources at the University of Pittsburgh, October 11-12, 2012.
25. Guest Lecturer for Hugen 2070: Bioinformatics for Human Genetics. “Introduction to Grid Computing.” August 31, 2012.
26. Co-Lecturer: Workshop on Introduction to Parallel Programming with OpenMP. University of Pittsburgh, May 1-2, 2012.
27. Presentation to Department of Biomedical Informatics. “High-Performance Computing at the University of Pittsburgh.” January 13, 2012.
28. Lecturer: Introduction to Linux, ENGR2403. University of Pittsburgh, Spring 2011.
29. Guest Lecturer for Phys 2274: Computational Methods. “A Brief Survey of the MPI Model of Parallelization.” December 16, 2010.
30. Co-Lecturer: Introduction to Collaborative Scientific Programming, ENGR2402. University of Pittsburgh, Spring 2010.
31. Co-Lecturer: Introduction to Parallel Computing. University of Pittsburgh, Spring 2009.
32. Presented seminar for Pitt CS Technology Leadership Initiative, a summer camp supporting high-schoolers from minorities typically underrepresented in computer science, 2009.
33. Reviewer for ACS *The Journal of Physical Chemistry* (2002-2006) and *Chemical Physics Letters* (2009-2010)

**(h) Collaborators**

Lillian Chong (University of Pittsburgh),

Lee Harrison (University of Pittsburgh)

Bruce Y. Lee (Johns Hopkins University)

**(i) Graduate and Postdoctoral Advisors:**

Post-Doctoral: Gregory A. Voth (University of Utah)

Post-Doctoral: Sharon Hammes-Schiffer (The Pennsylvania State University)

Ph.D.: Peter Rossky (University of Texas)