2017 COMP Division Election

Chair

Michelle Lynn Hall

I'm a computational chemist at Moderna Therapeutics, where I spearhead applying computational chemistry techniques to the frontiers of mRNA therapeutic design. I'm also the Program Chair for the Boston Area Group for Informatics and Modeling (BAGIM), an ACS COMP affiliate dedicated to computational chemistry education and professional networking. Prior to joining Moderna, I worked at Schrodinger as a Principal Scientist where I interfaced with end-users and developers alike, giving me broad knowledge of the unique challenges in our field. Immediately before, I completed my postdoc in the Computer Aided Drug Discovery (CADD) department at Novartis Institutes for Biomedical Research (NIBR) joint with Prof. William Jorgensen at Yale University. I completed my Ph.D. at Columbia University with Prof. Richard Friesner where I specialized in Density Functional Theory development and theoretical organic chemistry. I also lead Women in Science at Columbia, an organization dedicated to professional development, diversity, and inclusion in science, technology, engineering, and math.

Chair statement:

As Chair of ACS COMP, I would focus on three key areas: (1) strengthening the interaction with local sections and international chapters, (2) diversity and inclusion in the chemical enterprise, and (3) growing the scope of national meeting programming for the COMP technical division.

1. Local meetings provide important opportunities for networking with other local professionals. While vibrant local networking opportunities exist in hubs such as Boston, I hope to foster these networks in other local chapters outside of these central hubs. Additionally, we could simulcast scientific seminars that occur regularly at local chapters in the hubs to ACS COMP members globally, ensuring that all members can benefit from these professional development opportunities regardless of their physical location.

2. It is well established that diversity drives innovation. Therefore, I would work to create an inclusive community for our membership. This could be achieved via tighter integration with the Women Chemists Committee and events aimed at students, postdocs and early career scientists, such as postdoc breakfasts, organized mentoring initiatives, and daytime lunch and learns.

3. Since computational chemistry is inherently an interdisciplinary field, I'd strive to increase the amount of cross disciplinary programming with other divisions to benefit the professional development of ACS COMP members. Area for cross fertilization include biological chemistry, medicinal chemistry, chemical toxicology, and materials science

Thank you for your consideration. I look forward to the opportunity to serve as your ACS COMP Chair.

Veerabahu Shanmugasundaram

Veer Shanmugasundaram currently leads the Computational Analysis and Design (CAAD) group in Pfizer, Groton, CT. Veer joined Pfizer, Ann Arbor in 2003 through the Pharmacia acquisition and has worked in various disease areas. He is a coinventor of two clinical candidates in Dermatology for treatment of alopecia and acne and two candidates in Anti-Bacterials for the treatment of multi-drug resistant Gram-negative infections. His current research interests are in novel modalities and novel modes of action space. Veer received his Ph.D. from State University of New York at Buffalo and conducted post-doctoral studies at Pharmacia & Upjohn in Kalamazoo, Michigan. He is a Guest Lecturer at the University of Bonn, Germany and has published over 30 manuscripts and given over 30 invited lectures at various scientific conferences. He received the 2015 Bonn-Aachen International Center for Information Technology (B-lT) Lectureship Award granted by the Department of Life Science lnformatics, University of Bonn, Germany.

Veer has been an active member of the ACS and has been involved in COMP division for the past several years. He has contributed to the division's annual reports, volunteered time through mentoring and outreach activities, and served the division in various capacities - Alternate Councilor, Assistant Secretary, and Secretary. He also participates at regional meetings such as MARM and has contributed to panel discussions on "Computational Chemistry in the Undergraduate Curriculum: Past & Future" He has served on several ACS Awards, Nomination & Selection Committees and Journal Advisory and Review Boards.

Veer has organized numerous symposia at ACS meetings (co-sponsored with CINF, MEDI and MPPG divisions). He is a member of CINF and MEDI divisions in addition to COMP and has encouraged joint symposia and interactions between divisions. Recently he co-organized the 2015 CINF Herman Skolnik Award symposium honoring Prof. Jürgen Bajorath (with Rachelle Bienstock), the 2016 MPPG division Computational Biophysics symposium (with Kate Holloway), the 2017 COMP Cloud Computing symposium (with Jeff Blaney, Essam Metwally and Raul Alvarez). He also co-organized the 2017 CADD Gordon Research Conference (with Pat Walters)

that was held recently in Mount Snow, VT. Veer is also on the International Organizing Committee for the 22nd EuroQSAR meeting that will be held in Greece in 2018.

Chair Statement: I would like to build on COMP division's past successes and tackle the challenges the division faces in the years ahead with fundraising and thereby strengthen the division during my tenure. As a practicing industrial computational chemist and group leader, building the next-generation computational chemistry capabilities and talent is near and dear to my heart. I have been reaching out and interacting with other divisions in the ACS through my participation in awards nominations & selection committees and through symposia organizations. I have initiated strong collaborations with various colleges, universities, biotech and pharma both in the US and abroad in my role at Pfizer and through the ACS crosspharma leaders group.

The principal challenges the COMP Division faces are in the general area of funding and membership. The bellwether indicators include reductions in division membership, decline in industrial sponsors and contraction of the number of Councilors. With the industry in flux and academia facing unprecedented funding challenges, there is a need to identify, engage and inspire the next generation of computational chemists and researchers while retaining our strongest advocates and supporters.

If elected, I will focus on the following:

· Increase long term fiscal strength

· Stay more visible in advocacy and education

· Sustain membership by attracting and retaining division members

These could be accomplished in a few ways, such as:

· Enhancing fiscal strength of the division by identifying and sustaining sponsorships, reducing costs (where possible) and creating a long term strategic, fiscal plan

· Identifying and advocating research in pre-competitive space that will benefit both academia and industry (through ACS cross industry group).

· Leverage COMP division’s technical programming at national meetings, division awards and division outreach activities to catalyze interest in this space.

· Upgrading the COMP division website and being more visible in social media.

· Provide easier mechanisms for membership renewals, life-memberships through awards and necessitate (if needed) a few stringent measures such as requiring division memberships for ACS national meeting presenters, symposium organizers and COMP award recipients.

Working together we will overcome these challenges, establish close, mutually beneficial relationships within the community and with others across the divisions and build a strong future for the discipline.

Secretary

Katrina Lexa

Dr. Lexa has been an ACS member and COMP division member since 2005. She has been involved in coordinating the social media outreach for ACS COMP since 2015.

Katrina is currently at Denali Therapeutics, where she contributes to efforts to develop breakthrough therapies for neurodegenerative diseases. Prior to Denali, Katrina was at Merck as a computational chemist in Modeling & Informatics, focused on reaction modeling, enzyme design, and lead optimization within Process and Discovery Chemistry. She performed postdoctoral research with Prof. Matt Jacobson at UCSF, supported by her NIH Ruth L. Kirschstein Individual National Research Service Award. Katrina obtained her PhD in Medicinal Chemistry from the University of Michigan under the guidance of Prof. Heather Carlson. Her undergraduate degree is in Chemistry and Public Policy from Hamilton College, where she worked with Profs. George C. Shields and Karl N. Kirschner.

Councilor

Luke E. K. Achenie

Dr. Luke Achenie is a Professor of Chemical Engineering at the Virginia Polytechnic Institute and State University (Virginia Tech), in Blacksburg, Virginia. Prior to joining Virginia Tech in August of 2007, Luke was at the University of Connecticut (Storrs, CT). Luke has an M.S. degree in Applied Math (Carnegie Mellon University, Pittsburg, PA) and a PhD in Chemical Engineering also at Carnegie Mellon. Before joining academia, he did a three-year stint as Associate Research Engineer at Shell Development Company in Houston, Texas. At Shell he developed advanced process control and optimization algorithms for the oil refineries.

In Connecticut, Luke focused his research in computational modeling of chemical engineering systems with Mathematical Programming (optimization) as a core technology in his research. He developed algorithms in uncertainty analysis associated with chemical engineering processes. He also developed research interest in interval analysis strategies for solution of optimization models. However, he spent most of his effort in molecular modeling of liquid solvent and other liquid systems. Specifically he studied environmentally-benign refrigerant design, extractive solvents for chemical reactions and solvent effects on the morphology of pharmaceutical compounds such as ibuprofen. He currently has projects in computational materials design (membranes and composites) involving molecular modeling, BigData and machine learning. Luke's research activities led to an induction in the Connecticut Academy of Science and Engineering (CASE) in 2007. Luke has so far published over 160 archival papers and made several presentations.

The crucial role that chemistry plays in Luke's research led to his membership in ACS since 1996. Luke participated in conference attendance and presented papers but did not know the internal workings of ACS enough to lend a helping hand. This all changed when he joined the ACS/CMA (Committee on Minority Affairs) which he represented as a liaison on the ACS/CPRC. He is currently serving as COMP Representative to the MPPG (Multidisciplinary Programming Planning Committee) in which he was the 2015 Chair. In his involvement in MPPG, Luke proposed and pushed for the adoption of the Spring 2016 ACS Conference (San Diego) theme "Computers in Chemistry" which was well aligned with COMP. The COMP Division has a rich culture; however its membership is in decline or at best stationary; this has affected the number of councilor slots that are assigned to it. It is incumbent on all of us to get COMP to forge new alliances with other divisions within ACS, exploit the BigData and Machine Learning revolution to grow and evolve. Dr. Luke Achenie hopes to help in this effort by bringing fresh ideas from the outside. If elected as Councilor in COMP, Luke's background and his experience

as a one-year rotator as Program Director at the National Science Foundation will be brought to bear on the new role. In addition Luke will push to have new metrics that ensure equitable assignment of ACS resources to the divisions, especially smaller ones such as COMP. Luke is humbly asking for your vote.

On a side note, Luke is involved with the American Institute of Chemical Engineers (AIChE. He served on the coordinating body for Area 10a of the Systems Division from 1999 to 2002; in 2002 he served as the programming chair. Luke had and continues to have other roles within AIChE. For example he was on the CEOC Operating Council from 2006 to 2007. He was appointed to the Board of Trustees of AIChE (2010 to 2016) and is currently the International Committee Chair. Once again, Luke is humbly asking for your vote. Thank you.

Shanadeen Begay

My interest in networking within the ACS communities with a professional focus has been a life-long pursuit manifested in my personal and social collaborations with the Computers In Chemistry (COMP) Executive Board. As a member of the ACS Scholars program, I was given the opportunity to voice my passions for the indigenous communities of the Americas at the CMA Luncheon, and that solidified my support for the ACS Diversity work. I have been a Younger Chemists Committee Member and have received exposure to the goals and organizational structure of the national committees by participating as the Project SEED Liaison and submitting the Liaison reports. I have become the Northeastern Section Younger Chemists Committee Publicity Chair, and my goal has been to increase participation of local sections in the German Exchange Program, regional career fair, and the research conference. My objectives in the last 6 years as a member on the Diversity and Inclusion Advisory Board (D&I) and as a member on the Committee of Minority Affairs (CMA) was to work with both PHYS and COMP is to establish a network of scientists from all different areas of academic expertise and identify ways of integrating social values important to younger chemists into the chemical sciences.

One way to achieve this goal is contact at the five to ten universities, government labs, and industrial companies with self-identified younger scientists and establish a network of people dedicated to creating a mission statement that increases the younger chemists presence in the chemical sciences while preserving important relationships within those communities: Most importantly, there must be an activist component to this work that extends beyond just chemical sciences. COMP values can be expressed through the following mechanisms:

- Establish and maintain personal relationships with key leaders/representatives in the targeted community

- Facilitate mutual awareness by communicating relevant ACS goals/activities to the targeted groups, and by communicating the goals/activities of the targeted groups to relevant ACS units

- Identify mutual objectives that could be pursued in collaboration with the specific groups/communities

- Facilitate connections between the communities and ACS units to advance the opportunities identified

- Coordinate messages and efforts with relevant ACS units, develop action plans, and report semi-annually on progress to the ACS Diversity Partner Initiatives.

I appreciate that our division has a higher presence of industry members, which allows us to step outside the usual format of lectures. Thanks to their involvement, we benefit from a lot of outside support from industrial companies dedicated to our goal of recognizing scientific excellence.

I'm proud to say that COMP is a diverse division that represents ACS well when it comes to mentorship and progressive programming.

Academic Record: Northeastern University Post-doctoral Research Associate, Northeastern University, Boston, MA; 2015 Ph.D. with Computational Certificate, Chemistry Department, Boston University, Boston, MA; 2006 B.S.C.S. Northern Arizona University, Flagstaff, AZ; Minor: Mathematics; 2006 B.S. Chemistry, Northern Arizona University, Flagstaff, AZ.

Honors: Recipient of the Ruth L. Kirschstein National Research Service Award (10/2009-9/2012); Recipient of National Science Foundation Integrated Graduate Education and Research Traineeship for interdisciplinary graduate background and the technical, professional and personal skills needed to address the global questions of the future (08/2006–08/2007), NSF Biology Research Fellowship for Post-doctoral Associates (2015--2018).

Professional Position: Northeastern University, Post-doctoral Associate (2015-2018). Boston University, Graduate Student (2006-2015).

Christopher J. Cramer

I earned my A.B. from Washington University in St. Louis and my Ph.D. from the University of Illinois. My professional career began with four years of service as an officer in the United States Army, including combat duty in Operation Desert Storm, and then in 1992 I began my academic career at the University of Minnesota, where I am currently a Distinguished McKnight

and University Teaching Professor and also Associate Dean for Academic Affairs in the College of Science & Engineering. I am honored to have been recognized as a fellow by the American Chemical Society, as well as by the Alfred P. Sloan and John Simon Guggenheim foundations. I wrote the textbook *Essentials of Computational Chemistry, Theories and Models,* I designed (and continue to teach) a popular massive open online course, *Statistical Molecular Thermodynamics*, and I maintain a YouTube Channel with 150+ videos also teaching computational chemistry and thermodynamics. My research interests encompass the development and application of models that include condensed-phase effects on structure and reactivity, as well as the application of computational methods for catalyst and materials design, with special interest in fuel liquefaction, water splitting, oxygen activation, sustainable polymers, and chemical weapons remediation.

My commitments to our profession include having served as the Editor-in-Chief of *Theoretical Chemistry Accounts* for 15 years. I now continue to serve as an Associate Editor for the *Journal of Physical Organic Chemistry*, and I spent three years on the editorial advisory board for the *Journal of Organic Chemistry*. I spent multiple years as a board member for the Reaction Mechanisms Conference and a councilor of the International Society of Quantum Biology and Pharmacology. In service specifically to the American Chemical Society, I have organized many symposia for regional and national meetings, served on (and chaired) an ACS Awards committee, and from 1994-1996 I served as Chair-elect and Chair of the COMP Division itself, continuing involvement with Division leadership and the Executive Committee on an ad hoc basis after that.

I would consider it a privilege to represent the Division and its membership as a Councilor. I am especially interested in (i) communicating more effectively to the general public the important role that our profession plays in technology and everyday life, and *should* play in the development of relevant public policy, and (ii) ensuring that our Society recruits, sustains, and advocates on behalf of a diverse membership that brings to our profession a critical wealth of backgrounds and experiences.

Terry Stouch

Terry is past chair of COMP which includes responsibility for a year as chair elect and a year past chair and he has served for the last 2 years as an alternate councilor. For many years before that he participated in COMP Executive meetings as a contributor to COMP symposia, a number of which he has supported financially as Senior Editor-in-Chief of the Journal of Computer-Aided Molecular Design. As chair he worked to reduce costs, engage current and new

members, and increase value for the members. He has been member of the ACS and COMP for 35 years. During that time he organized, chaired, and funded numerous COMP symposia on a variety of topics.

Terry is Senior Editor-in-Chief of the Journal of Computer-Aided Molecular Design a position he has held since 2003. He has over 30 years' experience in drug discovery research in both large pharmaceutical companies (Bristol-Myers Squibb) as well as biotech (Lexicon Pharmaceuticals). His specialties include structure-based drug design, QSAR, force field development, data analysis. and software design and development. Since 2008 he has consulted on drug discovery and design and data evaluation and analysis. He consulted at length for the Protein Data Base. He is known for early studies in large-scale simulations of biological membranes.

He has been Adjunct Professor at the University of Kentucky, Duquesne University, and University of Maryland Baltimore and is a AAAS Fellow and an IUPAC Fellow. Terry has served on hardware and software advisory committees for the Pacific Northwest National Laboratories and is a member of two committees of the Pistoia Alliance. He was a member of the design team for the initial development of the LAMMPS simulation software

Ralph A. Wheeler

Ralph Wheeler became a Professor and Chair of the Department of Chemistry and Biochemistry at Northern Illinois University in July 2016 after six years in the same position at Duquesne University in Pittsburgh and 20 years as a professor in the Department of Chemistry and Biochemistry at the University of Oklahoma. Ralph received a BS degree in chemistry from Harvey Mudd College in 1982, a PhD in computational chemistry from Cornell University in 1988, and completed 2-years of postdoctoral training with Andy McCammon in 1989. Ralph spent his first sabbatical with Peter Kollman's group at UC-San Francisco in 1997-98, and a second sabbatical at the Scripps Research Institute in 2006.

Ralph Wheeler's current research spans computational biochemistry and materials chemistry, using quantum chemical, molecular dynamics, and QM/MM methods. They include implementing new methods of modeling radical reactions and adapting signal processing methods to analyze molecular dynamics simulations. His method development work is driven by applications, often in collaboration with experimentalists working to infer local structures from vibrational spectra of proteins or polymer melts, understand the structures and functions of electron transfer proteins, and design better ionically conducting polymers for battery applications. He has more than 75 publications in computational chemistry, many with experimental co-authors. Ralph has mentored 16 PhD/MS students and 30 undergraduate researchers. He is particularly proud of the many awards won by current and former co-workers,

including Fulbright, NIH, NSF, and National Research Council Fellowships, as well as an NSF POWRE Award (Professional Opportunities for Women in Research and Education).

Ralph has been an active ACS member for more than 35 years, was named a Fellow of the ACS in 2010, and believes that everyone should give back through service to the profession. He feels privileged to have served as Program Chair for the ACS Computers in Chemistry Division for four years, when the number of COMP presentations at national meetings grew from 170 to a then-record 492, Division officers secured corporate sponsorship for the symposium to present the ACS Award for Computers in Chemical and Pharmaceutical Research, and the Division created its first endowed symposium in honor of an eminent computational chemist. In addition, the Division initiated the "Emerging Technologies" symposium and secured corporate sponsorship for a regularly scheduled symposium. As the Division's Chair in 2007, he initiated long-range strategic planning in conjunction with ACS facilitators and began implementing the Division's new strategic vision. His service as a Councilor for the COMP Division during three terms has included service on the ACS Committee on Science and its Awards and Policy Subcommittees. He was recently asked to serve on an ACS Working Group to determine whether or not the Society needs a policy statement on immigration. Ralph believes that he can leverage his current position on the Governing Board of the Council for Chemical Research to benefit both the ACS and the CCR. He would be honored to continue serving the COMP Division members and would appreciate your vote!

Scott Wildman

Scott has been an ACS member since 1996 and a COMP Division member since 2001. He has been involved in organizing ACS national meeting programming since 2010, and served as Assistant Program Chair from 2011–2015.

After receiving B.S. and M.S. degrees in Chemistry from Clarkson University, Scott earned a Ph.D. in Medicinal Chemistry from the University of Michigan in 2001, working for Prof. Gordon Crippen. He worked as a computational chemist for Pfizer for 7 years in Ann Arbor, MI and Cambridge, MA, applying a wide variety of computational techniques across number of different therapeutic areas. In 2008, he moved to Washington University in St. Louis in a collaborative role designed to move academic drug discovery projects toward the clinic. Scott is now at the University of Wisconsin, Madison, where he continues to pursue drug discovery projects as part of the UW Carbone Cancer Center.

His current projects include cancer treatments and antimicrobial therapies as well as new computational techniques, work that is supported by the NCI and NIAID, the UWCCC and the UW College of Agriculture and Life Sciences.