2018 ACS COMP Biographies and Statements

Chair 2020 (Chair-elect 2019)

1) Luke Achenie, Candidate for Chair of COMP

I am a Professor of Chemical Engineering (with a courtesy appointment as Professor of Health Sciences) at the Virginia Polytechnic and State University ("Virginia Tech"). The subjects I liked most in high school were mathematics and chemistry. It is not surprising that I got my BS in Chemical Engineering at MIT (Cambridge, MA) in 1981, followed by an MS in Engineering Science at Northwestern University (Evanston, IL), MS in Applied Mathematics at Carnegie Mellon (Pittsburgh, PA) and finally a PhD in Chemical Engineering also at Carnegie Mellon in 1988. After a three-year stint at Shell Oil at Westhollow (Houston, TX) I followed my instincts into academics. At the University of Connecticut (Storrs, CT), I rose through the ranks from Assistant Professor to Professor of Chemical Engineering in 2004. In 2007, I moved to Virginia Tech (Blacksburg, VA) where I have been since that time. I was elected into the Connecticut Academy of Science and Engineering (CASE) in 2007. I also became a fellow of the American Institute of Chemical Engineers (AIChE) in 2014.

My research is computational and a large portion of it is in multi-scale multi-physics molecular modeling that involves MD and DFT calculations. Specifically I do molecular dynamics modeling of membranes (for separation of gases), Chemical Vapor Deposition modeling and computational modeling of drug transport in the GI tract as well as across the blood brain barrier. The research also involves a new multi-agent approach for coupling molecular level molecular dynamics with macro level (i.e. continuum based) computational fluid dynamics/general particle dynamics. The MD calculations will provide quantities such as viscosity and diffusion constants to the fluid dynamics simulation at discrete times. In turn the performance of the fluid dynamics simulation and the MD trajectories could be used to develop a machine-learning algorithm that would provide predicted MD trajectories to speed up the MD simulation. In summary the approach will bridge the time and space scales of molecular level MD and continuum scale modeling. In the area of optimization (aka mathematical programming), I have done work in multi-objective optimization under model uncertainty, global optimization using branch and bound and interval arithmetic concepts. I have published over 160 archival publications. I am a member of a number of professional organizations, including ACS (since 2001), AIChE and SIAM.

Why should you consider me for COMP Chair? Consider the following experiences. From 2004 to 2007 I served as the Director of Computing Resources at the University of Connecticut School of Engineering. From January 2012 to January 2013, I took a year leave of absence from my academic job to serve as a Program Director within the CBET (Chemical, Bioengineering, Environmental, and Transport Systems) Division of the National Science Foundation (Arlington, VA). I previously served as an executive committee member of the ACS/CMA (Committee on Minority Affairs). For the past six years I have been the COMP representative to the MPPG (Multidisciplinary Program Planning Group – a group that selects themes for ACS National Meetings); I am a previous chair of the Thematic Programming sub-Committee and the 2015 Chair of MPPG. Through attending most COMP Division Executive Meetings since 2006, I have come to know the division quite well.

If elected as COMP Chair I will encourage COMP to do a significant portion of its programming (up to 20 %) at the interfaces supported by MPPG; through such interfaces, we can grow COMP membership and exposure to COMP as I truly believe that COMP has an impact on several areas of ACS and is poised to have an even greater translational impact on all areas of ACS. The sheer size of ACS and the number of divisions provide countless opportunities to serve and be served by the richness of the diversity of people, the diversity of opinions (both scientific and social). I believe COMP should exploit these realisms. Thank you.

2) Seonah Kim – Bio and Chair Statement

I'm a Senior Scientist at the US National Renewable Energy Laboratory (NREL) in Golden, CO, since 2011 leading various computational chemistry projects related to energy, fuel and catalysis. Working in multidisciplinary teams of theoretical and experimental chemists and engineers, we have used mechanistic studies into of a variety of catalysts, both biological and inorganic, to design catalysts for biochemical and thermochemical conversion processes. I have expanded our research area to develop a fuel property prediction tool using machine-learning and quantum chemistry.

Previously, I specialized in both quantum mechanical methods and molecular dynamics simulations - conducting postdoctoral research at UCLA with Prof. Ken Houk on de novo enzyme design, and graduate work at the University of Florida with Prof. Adrian Roitberg studying protein simulations.

Having been involved with chairing program sessions and poster judging for a number of years, I joined the ACS COMP executive committee in 2016. As editor of the ACS COMP Newsletter I have gotten to know the people of COMP and the workings of our division. During this time the division has looked to support our community in several ways – with greater undergraduate programming, student-mentor lunches, a "Women in COMP" symposium (plan in 2019), and recognizing postdoctoral excellence.

As Chair of COMP, I bring organization, energy and an inclusive perspective. My plan as Chair is to continue to build the COMP community to be one that elevates the visibility of the field and one that facilitates networking and mentoring. These are priorities I want to continue and improve:

- Alongside academia and industry, national laboratories and government agencies are a significant career destination for our members – I plan to increase engagement at COMP activities to provide opportunities for collaboration and connectivity with graduate student and postdoctoral associates.

- I've worked to make the COMP newsletter a helpful way to keep up-to-date with divisional activities for those unable to attend ACS meetings. I plan to use the COMP website to further engage with the broader (and international) community and to provide useful resources.

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

Treasurer (2019-2021)

Lewis Whitehead

Lewis Whitehead is a computational medicinal chemist at Nimbus Therapeutics in Cambridge, Massachusetts. Having recently completed 19 years at Novartis, Lewis has worked on drug-discovery projects that have delivered three small molecules to human clinical trials for arthritis, cancer & infectious disease. He is the co-author of 21 research publications & has co-inventor credit on 7 patents. A chemistry graduate of the University of St. Andrews, with a Ph.D in Chemical Biophysics from the University of Southampton, Lewis has now been an ACS member for 13 years & is currently the Treasurer of the Division. During this time as treasurer, he has focused on more reliable & efficient payment processes. He has recently been granted an Innovative Project Grant for an upgrade to the Division's communication streams & generated the idea for a social networking event on the Saturday evening prior to the beginning of the national convention, which he also organizes. A focus for the treasury role over the next few years would be increased fundraising & involvement in strategic planning. He is a Life Member of the Kenya Chemical Society, serves on the Board of Directors of Boston based non-profit Seeding Labs, is a member of the ACS Committee of Science & is a United States National Committee member for IUPAC.

Councilor III (2019-2021)

Christine Aikens

I am a Professor of Chemistry at Kansas State University. My research focuses on many aspects of computational materials science, including modeling of gold and silver nanoparticle optical properties and chemical reactivity and investigation of metal oxide catalytic properties.

I have been a Councilor for COMP for the last three years. I have really enjoyed helping with the Materials Science programming for National ACS meetings, and plan to continue to do this. As a Councilor, I have also become involved with the Meetings and Exhibitions (M&E) Committee. My goal with this committee is to improve the experience of COMP members at National ACS meetings by improving poster sessions, meeting locations (especially to reduce the use of hotels… wish me luck!), and related matters. (Also, if you have other suggestions regarding the meetings, feel free to let me know!) I am currently an Associate Member of M&E. If selected as a Councilor for the next three years, I would hope to serve COMP as a Full (voting) Member of M&E.

My interest in theoretical chemistry began in my undergraduate years at the University of Oklahoma. After taking quantum mechanics courses, I realized that I loved electrons. I was fortunate to start working with Ralph Wheeler studying mechanisms of Diels-Alder reactions. Angela Wilson, who was a visiting research scientist in the group, suggested that I pursue method development in graduate school. After a summer research experience in 1999 with Don Truhlar at the University of Minnesota, I was hooked!

I entered my graduate studies in 2000 at Iowa State University working with Mark Gordon. While there, I was fortunate to be able to study a wide variety of research, from parallel implementation of various open-shell perturbation theory methods, to solvation of glycine, to magnetic properties of titanium compounds. After completion of my Ph.D. in 2005, I

moved to Northwestern to do a postdoc with George Schatz. It was there that I discovered the joy of studying the spectroscopy of metal nanoparticles.

I began my independent career at Kansas State University in 2007 as an Assistant Professor, and was promoted to Associate Professor in 2012 and Full Professor in 2015. I love working with students and think that it is one of the most valuable things that we can do in academia. Since my undergraduate research figured prominently in my career choices, I try to go out of my way to encourage undergraduates to participate in research experiences. If this research is computational, even better!