

2016 COMP Election Bios

Chair

1) Patrick Lee

Patrick Lee is currently an Investigator at the Novartis Institute for Biomedical Research in the computational chemistry group based in Emeryville, CA.

Prior to Novartis, Patrick was at Eli Lilly & Co in San Diego executing fragment strategies for various structurally enabled targets. He ended up at Eli Lilly upon its acquisition of SGX Pharmaceuticals in 2008. At SGX, he was a key contributor on a kinase project that delivered a clinical candidate for cMet. Patrick carried out his NIH Kirschstein-NRSA postdoctoral fellowship at Yale University with Professor W. L. Jorgensen and obtained his Ph.D. under the guidance of Professor K. N. Houk at UCLA where he received a first year academic/research award. He received his undergraduate degree in chemistry from Pomona College in 1998.

During Patrick's tenure as an alternate councilor in COMP (2009-2015), he has focused on helping COMP members network with other COMP members and other ACS members via social network sites. Patrick created the ACSComp LinkedIn group as well as the Twitter handle @ACSCOMP on behalf of the COMP division to aid this purpose. Patrick was also an associate in the CPRC (committee on public relations and communications) for two terms (2011, 2012) and is currently a member (since 2014). Patrick also participates in the bay area COMP Together events and works with local champions to generate topics for local networking events. Patrick has been a member of the ACS since 1998.

Chair

2) Maria Nagan

Bio and Chair Statement

I am a Professor of Chemistry at Adelphi University in Garden City, NY (2013-present) and wrapping up my term as Chair of the department. Previous to Adelphi, I was a Professor and Director for the Office of Student Research at Truman State University, a primarily undergraduate institution and honors college for the state of MO. I earned my B.A. from Grinnell College and my PhD with Chris Cramer at the University of Minnesota. I also spent a sabbatical working with Darrin York in 2008-2009. My research uses both quantum mechanical methods and molecular dynamics simulations to better understand RNA structure and peptide-RNA recognition.

I have been a member of COMP for a number of years but only recently, in the last year, have I become more involved. I was brought in to help with undergraduate programming. For the last two national meetings, I've coordinated undergraduate poster judging in the CHED-COMP and COMP sessions. In collaboration with Ed Sherer (current Chair), I also organized the first COMP Undergraduate Workshop, which consisted of a mini-tutorial in QM and MD methods and a career panel with representatives from industry, scientific publishing and academia.

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:

- If you can't make it to the ACS meeting, our COMP newsletter will keep you in the loop about goings on but also opportunities for continued professional development.
- Successful COMP Together social activities right before the meeting allow local COMP scientists to partake in COMP activities without having to attend the whole ACS meeting.
- We plan to continue a COMP Undergraduate Workshop every Spring meeting.
- We've talked about making our website a hub for tutorials and COMP-related science information.
- As Chair, I'd also like to find small, tractable opportunities so COMP members can become involved in the division. With some planning and communication, I think people will be happy to help.

Thanks for reading this far. ☺ Please vote for me for Chair.

Chair

3) Veerabahu (Veer) Shanmugasundaram

Veer Shanmugasundaram currently leads the Computational Analysis and Design (CAAD) group at the Center of Chemistry Innovation & Excellence at Pfizer, Groton, CT. Veer joined Pfizer, Ann Arbor in 2003 through the Pharmacia acquisition and has worked in various disease areas. He is a co-inventor 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 at Pfizer are in expanding target space through novel modalities and mechanisms such as covalent inhibitors, oral cyclic peptides, chimeric agents and drug conjugates, targeting new protein families. He is also interested in improving design effectiveness by innovating in large scale SAR visualization & analysis and improving probabilities of success in medchem campaigns. Veer 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. Veer received his Ph.D. (Medicinal Chemistry) from State University of New York at Buffalo and conducted post-doctoral studies at Pharmacia & Upjohn in Kalamazoo, Michigan.

Veer has been a long standing active member of the ACS and has been involved in COMP division activities for the past several years and is familiar with COMP division's strengths, challenges, aspirations and objectives. 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 has organized numerous symposia at ACS meetings (co-sponsored with CINF, MEDI and MPPG divisions) and has actively been involved in COMP programming. 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 (with Rachelle Bienstock) and the 2016 MPPG division Computational Biophysics symposium (with Kate Holloway). Veer has raised sponsorship money for all symposia that he has organized thereby providing waivers of registration fees and/or travel grants to students, post-docs and faculty members. He has served on several ACS Awards, Nomination & Selection Committees and Journal Advisory and Review Boards. Recently he was elected as the Program Chair of the prestigious 2016 CADD Gordon Research Conference.

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 membership, fundraising, and talent retention 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 cross-industry 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.
- 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.

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

Councilor

1) Emilio Xavier Esposito

In all aspects of Emilio's Councilor and Committee work, he makes decisions serving the best interests of the COMP membership. Emilio would be honored if the COMP Division membership would once-again select him to represent the COMP Division as a Councilor.

Emilio has been active in the COMP Division since 2006 serving as an Alternate Councilor (2007-2008) Councilor (2008-present), Assistant Programming Chair (2006-2010) and Programming Chair (2011-2015). In addition to his work within the COMP Division, Emilio is a member of the Technical-Programming sub-committee (2009-present) for the Meeting & Expositions committee, an Associate Editor of the ACS Presentations on Demand (2013-present) and a former member of the PACS Advisory Board (2010-2015). Emilio has been nominated to serve on the Committee on Committees starting in the fall of 2016.

Emilio is a Data Scientist at exeResearch LLC and earned his B.S. and Ph.D. from the Department of Chemistry and Biochemistry at Duquesne University. His research interests include: QSAR and QSPR methodologies and paradigms, structure-based drug design, and exploring potential ligand-receptor interactions to design better scoring functions.

Councilor

- 2) **Peter C. Jurs: Division of Computers in Chemistry** (Central Pennsylvania Section). Pennsylvania State University, University Park, Pennsylvania.

Academic Record: Stanford University, B.S., 1965; University of Washington, Ph.D., 1969.

Honors: ACS Fellow, 2009; Presidential Award for Excellence in Academic Integration, Penn State, 1998; ACS Award for Computers in Chemistry, 1990; Barbara and Dean Martin Lecturer, University of South Florida, 2000; Archer Lecture in Organic and Medicinal Chemistry, Rensselaer Polytechnic University, 2001; American Association for the Advancement of Science Fellow, 1987; Merck Award for Faculty Development, 1970.

Professional Positions (for past ten years): Pennsylvania State University, Emeritus Professor, 2005 to date; Professor, 1978-05; Assistant Head for Undergraduate Education, 1995-04; Acting Department Head 1998-99.

Service in ACS National Offices: Council Policy Committee, 2012-present; Committee on Nominations and Elections, 2006-11; Committee on Publications, 1997-04, Committee Associate, 2005-08; Society Committee on Publications, 1991-97; Society Committee on Chemical Abstracts Service, 1982-90; Committee on Membership Affairs, Committee Associate, 1979; Advisory Board, *Journal of Chemical Information and Modeling*, 2005-07; Advisory Board, *Journal of Chemical Information and Computer Science*, 2004, 1977-85; Advisory Board, *Journal of Medicinal Chemistry*, 1994-98; Advisory Board, *Analytical Chemistry*, 1988-90.

Service in ACS Offices: Member of ACS since 1965. *Division of Computers in Chemistry:* Councilor, 1997-08, 1979-93, 1997-2015; Alternate Councilor 1994-96. *Central Pennsylvania Section:* Secretary, 1971.

Member: American Association for the Advancement of Science, Fellow. *ACS Divisions:* Analytical Chemistry; Chemical Education; Computers in Chemistry, and Professional Relations.

Related Activities: Supervised 57 graduate chemistry degrees (19 M.S., 1 D.Ed., 37 Ph.D.); co-author of general chemistry textbook *Chemistry: The Molecular Science*, 4th Edition, Brooks/Cole; approximately 270 research publications; Editorial Advisory Board, *Chemical & Engineering News*, 2000 to 2004; *Consultant to:* Los Alamos National Laboratory; Molecular Design, Ltd.; W.R. Grace; Beilstein Institute; Chemical Manufacturers Association; Chair, Organizing Committee, *3rd Symposium on Computer-Enhanced Analytical Spectroscopy*, Snowbird, Utah, June, 1990; Gordon Research Conference on Computer Aided Drug Design, Chair, July 2005, Program Chair, July 2003; National Science Foundation, Program Director, Chemical Analysis, 1983-84; *Analytica Chimica Acta*, Editorial Board, 1977-88; *ChemTracts, Analytical and Physical Chemistry*, Contributing Scholar; Member-at-Large, Section Committee on Chemistry of the AAAS, 1999-03;

Councilor

3) Scott Wildman

Dr. Wildman 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.