2019 COMP Election Biographies & Statements

Chair 2021 [Chair-elect '20]

Two candidates:

- Petrina Kamya
- Daniel Ortwine

Councilors [three-year term] & Alternate Councilors

Nine candidates: *(candidate with the most votes will become councilor III, candidates with second-most thru fourth-most votes will become alternate councilors)*

- Luke Achenie
- Kira Armacost
- Marco DeVivo
- Emilio Esposito
- Emilio Gallicchio
- Vanda (Vassiliki-Alexandra) Glezakou
- Daniel Mainz
- Robert Paton
- Qin Wu

- Petrina Kamya Chair 2021 [Chair-elect '20] Nominee

Bio:

Petrina Kamya was born in Kenya and at 16, she moved to Canada as an international student. A few years later, she obtained a Bachelor's degree in Biochemistry, and a PhD in Computational Chemistry from Concordia University in Montreal. For the last nine years, she has worked in the life sciences software industry (molecular modeling) and in healthcare consulting. In her current role at Certara, she uses real world data to investigate the effectiveness of drugs from a clinical, economic and epidemiological perspective. In addition, she works to make new drugs more accessible to those who need them. Petrina has been an ACS member for over 10 years. She previously served as assistant to the secretary in the COMP division and was involved with the CCG excellence awards for graduate students in the COMP division. She also set up the CCG graduate student awards in the MEDI division.

Statement:

Some of the most impactful professional and personal experiences Petrina has had are those that involve inclusion and diversity. Her goal as ACS COMP chair would be to bring those two attributes to the COMP division. There are 32 divisions at the ACS, but very little interaction between them. By promoting more interaction between COMP and other divisions, we will learn from each other, increase our exposure and understand just how interconnected we are. Let's grow together by being more inclusive and diverse.

- Dan Ortwine Chair 2021 [Chair-elect '20] Nominee

Bio:

I am currently a Principal Scientist in the Computational Drug Discovery group within Discovery Chemistry at Genentech. I received a bachelor's degree in Chemistry from the University of Michigan in 1976 and joined Pfizer shortly thereafter. After progressing to a Research Fellow position in a 31-year career, I left in 2007 to join Genentech, where I am actively engaged in supporting therapeutic project teams using computational chemistry and cheminformatics techniques. My expertise is in structure-based drug design, pharmacophore modeling, and QSAR around ADME endpoints. My interests lie in virtual screening, rational de novo design of novel ligands, protein-water interactions, and in delivering computational models to chemists' desktops to permit widespread use. I have organized multiple symposia in the COMP, CINF, and MEDI Divisions at ACS National meetings on topics such as docking and scoring, high throughput screening triage, model domain applicability, exploiting unusual protein-ligand interactions in drug design, harnessing the world's literature, and predicting toxicity. Currently I am co-organizing two day-long symposia on Computational ADME and Data Visualization at the upcoming 258th ACS National meeting in San Diego. I been an active participant in several COMP Executive sessions as an interested observer, as well as participating in the COMP mentor lunches at ACS National Meetings.

Candidate statement:

Personally, I continue to feel passionately about the role the COMP Division can play in guiding the evolution of computational science, and as such am excited about the opportunity to help guide the Division into supporting the next era of computing. The field continues to make great strides advancing the state of the computational art. Free energy perturbation calculations, crystal structure prediction, and AI-assisted force field development are but a few of the fields that are rapidly advancing. It is truly an exciting time to be a computational chemist! At Genentech, and at multiple conferences, I have been exposed to many academics and companies in this area and can bring my experience and insight gained to the Division.

The explosion of machine learning and AI technology coupled to the availability of large databases reminds me of the days of combinatorial chemistry, high throughput screening, and file enrichment, all of which promised to revolutionize drug discovery. These latter technologies and approaches have since settled down to become useful paradigms in the drug discovery process. The promise is clearly there for AI to deliver predictions not obtainable with 'conventional approaches'. The COMP Division is perfectly positioned at the nexus of these new technologies, and as such our members have a tremendous opportunity to play a central role in sorting the hype from the reality of AI in chemistry by staging timely symposia and webinars.

Obviously, I bring a large pharma industrial experience to the table, but I will not neglect the academic side of the Division. There must be a balance of presentations and activities from both industry and academia to effectively advance the field. I will work to ensure this balance is maintained in all Division affairs from officer membership to programming at conferences. Equally important is the diversity and inclusiveness of our membership, as such I will look actively engage and maintain outreach programs to maximize representation. At past ACS National meetings, COMP Division symposia have often been staged at hotels remote from the convention center, affecting attendance and visibility. As there is frequently substantial overlap in programming between COMP and other Divisions such as MEDI, CINF, and PHYS, I will work with the ACS to ensure our presentations are as proximal as possible to other Divisions with which we share science.

❖ Luke E. K. Achenie (Councilor Nominee)

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. Luke is currently an Alternate Councilor. 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.

❖ Kira Armacost (Councilor Nominee)

I am a computational chemist at Merck & Co., Inc., in West Point, PA. I completed my undergraduate degree in chemistry at the University of Tampa in 2007, and then received my Ph.D. at Auburn University in 2013. During my Ph.D., I studied theoretical organic chemistry under Dr. Orlando Acevedo, and identified the basis of the "on water" effect that certain pericyclic reactions like. I also performed molecular dynamics calculations to understand the mechanism of alkanesulfonate monooxygenase. I furthered my education with a postdoctoral fellowship at the University of Michigan under Dr. Charles L. Brooks, III, where I studied free energy calculations in the form of multi-site lambda dynamics. It was there that I fully developed my passion for drug design. I have been at Merck & Co., Inc, for the last three years working in the area of molecular modeling for discovery chemistry efforts. I actively work on projects supporting many therapeutic areas, and am still working on free energy calculations both in methodology development and application.

I have been the chair of the Journal of Chemical Information and Modeling (JCIM) Early Career Board (ECB) for the last year, and have published a perspective in JCIM describing the transition from academia into industry. I have been involved in promoting JCIM, organizing meetings for the ECB, and being a guest editor for an upcoming special issue. I am also active in the computational community in the Mid-Atlantic region. I am one of four organizers for the Mid-Atlantic Computational Chemistry group. We host yearly symposiums, and we just recently organized one with the New York Area Group for Informatics and Modeling (NYAGIM) in New York City in April. I was the representative for MACC at the most recent ACS COMP strategic planning meeting, where many local "AGIM" groups were represented. I am also an advocate for STEM related disciplines, and have volunteered locally at #girlSTEM, Discover your Future and iSTEAMM events for girls and boys within Bucks and Montgomery Counties in PA. I am also one of the organizers for the Fall ACS COMP symposium Women Make COMP. I have been a member of the ACS COMP community for ~10 years, and am excited for the potential opportunity to serve as a Councilor for the Division.

❖ Marco DeVivo (Councilor Nominee)

I am Director of the Molecular Modeling and Drug Discovery Laboratory at the Italian Institute of Technology (IIT) in Genoa (Italy). After a master's degree in Chemistry and a PhD in Pharmaceutical Chemistry from the University of Bologna (Italy), I moved to the United States in 2004. There, I worked for three years as a postdoctoral fellow under the supervision of Prof. M. L. Klein at the University of Pennsylvania in Philadelphia (USA). During this time, I attended ACS meetings and regularly presented my work at ACS Comp Division sessions. In 2007, to learn more about drug design and discovery, I joined the structure-based drug design group at Rib-X Pharmaceuticals (now Melinta Therapeutics, New Haven, CT, USA), working as a computational chemist while collaborating closely with Prof. Jorgensen's group at Yale. In 2009, after five fruitful years in the USA as a researcher in academia and industry, I joined the newly established Department of Drug Discovery and Development (D3) at IIT. This gave me the opportunity to start and lead my own laboratory at a top European institution.

Since the start of my career, I have been fascinated by the structure, dynamics, and catalysis of chemical systems. My goal is to advance our understanding of the general principles that control molecular recognition and catalysis, and to use this information to design intelligent nanosystems and inhibitors as drugs, particularly to fight cancer and neurodegeneration. In my group, we pursue this goal by integrating computational and medicinal chemistry with structural and biochemical data. The American Chemical Society (ACS) recognized my contribution to using multiscale simulations to elucidate the enzymatic processing of nucleic acids, presenting me with the ACS COMP OpenEye Outstanding Junior Faculty Award at the 253rd ACS National Meeting in San Francisco in 2017.

I am tremendously grateful for my years in the US, where I learnt so much about conducting research in top-level scientific environments. During those years, I built an international network of collaborations that is still at the center of my research activities. Indeed, since my return to Europe, I have maintained these lively and fruitful connections with colleagues in the US, visiting the US several times a year, and regularly participating in ACS meetings. I have been an active ACS member since 2004. I serve on the Editorial Board of the *Journal of Chemical Information and Modeling*, which is published by the ACS. I also participate in the ACS COMP Executive and Programming meetings at every ACS national meeting. This has allowed me to meet with members of the Executive Committee of the ACS COMP Division, and actively participate in the agenda and discussions.

I am honored and proud to be considered for a position as Councilor of the ACS COMP Division. It would be a great privilege to represent the Division and its membership in this role. My enthusiasm and motivation are connected to the numerous activities that link my work with ACS events and initiatives. In addition, at Executive Committee meetings, I would use this role to add a European perspective to discussions about the Division's activities. For example, I recently promoted the ACS COMP Division's involvement in scientific events (conferences, workshops, etc.) in Italy and other European countries. This involvement could attract new members and strengthen the connection between computational chemistry events and activities in America and Europe. I believe that these initiatives will broaden the ACS COMP Division's international impact, consolidating and further developing the network of connections between the Division and European scientists, including young students. Ultimately, this would benefit the professional development of ACS COMP members and the progress of the ACS COMP Division and membership in Europe. If given the opportunity, I will do my very best as a committed Councilor to represent and safeguard the interests of the ACS COMP Division. Thank you very much for your vote!

❖ Emilio Xavier Esposito (Councilor Nominee)

In all aspects of Emilio's Councilor and Committee work, he strives to make decisions that will best serve the 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 has been active on several national ACS committees. He was elected to the Committee on Committees (ConC) in the fall of 2016 and is currently chair of ConC's subcommittee on Diversity and Inclusion. Other committee work includes the Technical-Programming sub-committee for the Meeting & Expositions committee (2009-2016), Associate Editor of the ACS Presentations on Demand (2013-2017), and a member of the PACS Advisory Board (2010-2015).

Emilio is a Computational Chemist and Data Scientist at exeResearch LLC and Editor of the *Journal of Molecular Graphics and Modelling*. He 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, exploring potential ligand-receptor interactions to design better scoring functions, and demographic analysis of ACS divisions and members.

❖ Emilio Gallicchio (Councilor Nominee)

I am an assistant professor at the Department of Chemistry at the Brooklyn College of the City University of New York. My research interests range from statistical thermodynamics and molecular biophysics to high-performance computational modeling. My recent research focuses on the free energy modeling of protein-drug binding and macromolecular molecular recognition phenomena. More information about my research and educational activities is at compmolbiophysbc.org.

I have been engaged with the computational chemistry community for many years. I have been a member of the ACS and COMP since 1994. I have greatly benefited by COMP programs over the years, both as a participant and moderator of COMP symposia and as a recipient of a COMP award. I am looking forward to the opportunity to contribute more actively to the continuing success and strength of COMP. As councilor. I pledge to serve the Division in any way that is deemed useful, from day to day duties to the development and evaluation of new programs. I am interested specifically in the furthering of programs that emphasize interdisciplinarity and that highlight the unique position of computational modeling at the crossroads of theoretical chemistry, molecular physics, and information science.

I have started my independent academic career relatively late when I joined the Department of Chemistry at Brooklyn College and the Graduate Center of CUNY in 2013. Our Computational Molecular Biophysics Lab at Brooklyn College is a small but productive, diverse, and collaborative research hub for graduate and undergraduate students. I am the recipient of an NSF CAREER award (2018), of the Brooklyn College Levy-Kosminsky Professorship in Physical Chemistry (2018), of the Henry Wasser Award from the CUNY Academy for the Humanities and Sciences (2017), and of the NVIDIA GPU Best Poster Award from COMP in 2017. My graduate formation and early research at Columbia University have been in the field of theoretical chemical physics followed by postdoctoral studies at Rutgers University in computational biophysics, where I also served as associate director of the High-Performance Computing Center. In the early 2000s I was part of a small team of scientists who contributed to the founding of Schrodinger LLC, now a major provider of drug discovery software to pharmaceutical companies worldwide.

The experiences I have collected in the twist and turns of my career path, which started with theoretical research, intersected the pharmaceutical software industry, and is now complemented with chemical education at the undergraduate and graduate level, will hopefully bring unique perspectives to the COMP community. I humbly ask for your vote to serve as COMP councilor. Thank you.

❖ Vassiliki-Alexandra (Vanda) Glezakou (Councilor Nominee)

A native of Greece, I received my degree in Chemistry for The National Kapodestrian University of Athens. I wanted to be a Chemist from a very early age, and although I did not quite realize it then, my thoughts of Chemistry always involved spinning electrons and nuclei. It was no surprise that I upon graduation, I pursued a degree in Theoretical and Computational Chemistry. My graduate pursuits led me first to Iowa State University where I obtained my PhD, and then to University of California San Diego for a post-doc. In 2003, I accepted a Research Scientist position at Caltech with the late Prof. Kupperman. Shortly after that however, I was offered a staff scientist position at the Pacific Northwest National Laboratory (PNNL), where I have worked ever since.

Since my arrival at PNNL, I expanded my skills beyond quantum chemistry to include molecular dynamics methods. The group I currently co-advise includes about 12 post-docs, international visiting scientists and junior staff. Our work covers the areas of Catalysis, Separations, both fundamental and applied, the development of CO_2 capture solvents, or design of materials with tailored properties. In all these efforts, we work very closely with our experimental colleagues, which has given me a broader perspective on challenges that scientist face, regardless of their specific discipline.

I am currently one of the Editors of Nature, Scientific Reports, a regular author and reviewer for the ACS journals and have organized/co-organized several symposia at the National ACS meetings. I served as the Chair of the ACS Richland Chapter for 2017 and although I enjoyed my tenure at the local level, I feel ready to help promote our Society's goals and make the wonderful world of Chemistry even more accessible to all, but particularly younger people and aspiring future scientists. As one of the Coaches of Team Battelle, I have had the unique opportunity to coach math and sciences for several years now and witness how our kids minds can grow in the STEM areas under proper guidance. As a mother of a freshman, it delights me to no end to see how my daughter relishes to learn about quantum mechanics and Bell's inequalities and planning a future that does involve the science that I love so much.

I would be honored to serve as a Councilor of our Division and work alongside the leadership team to help make what we love more accessible to the general audience, especially younger generations, and help draw a more tangible picture where science clearly enables great technologies that make our everyday lives better and hopefully keep our world safe for the future.

❖ Daniel Mainz (Councilor Nominee)

I am a Senior Scientist at Schrödinger where I have been for nearly twenty years in various roles: development of QM, MD, docking, and cheminformatic applications, as well as project management. Nowadays I am happiest focussing my efforts on working with users of our applications leveraging my scientific and technical experience.

As a Councilor of ACS COMP, I hope to champion several causes about which I am passionate, including:

- **Novel ways to engage and support members**

  In my current role at Schrödinger, I interact with undergraduates at small colleges lacking large IT resources and expertise, renowned professors and industrial researchers with large budgets, and everybody in between. Good ideas can come from anywhere. With computational power ever increasing, and high-quality applications and API's becoming cheaper or even open-source, I strongly believe that our division must be proactively inclusive for all its members and affiliates, and help all chemists realize their potential, through travel grants, mentoring, software access, investments in online courses, and any other good ideas any of us can promote.

- **Equity, diversity, inclusion, and awareness**

  Diversity and inclusion in membership, speaker invitations, and publication opportunities are vital, not just to today's women and underrepresented scientists, but to the next generation as well. At every stage of my own career, I have seen too many talented people leave our field due to self-doubt, family obligations, inhospitable cultural bias, and financial fears. I've been a passive member of ACS COMP for many years, consistent with my tendencies to listen and advise others, but increasingly I understand that lasting change requires the active efforts of us all.

- **Greater engagement with other chemistry disciplines**

  As councilor, I hope and expect that I can continue to empower all of you, improve the reach and exposure of our division, and strengthen our ties with other divisions. Rather than passively await organic, inorganic, polymer, materials, medicinal and other chemists come to us with their questions and concerns about computational methods, let us reach out to them and show how our experience furthers their research.

Like you, I am excited to see what is to come in our field and share your hope that everyone has the opportunity to contribute to and benefit from the best inventions and applications. I look forward to serving as your Councilor and thank you for your vote.

❖ Robert Paton (Councilor Nominee)

I am an Associate Professor in the Department of Chemistry at Colorado State University. My research group uses computational chemistry to model and predict the outcomes of chemical reactions and to address the challenges of efficiency and selectivity inherent to synthesis. This work has involved multiple collaborations with experimentalists and computational chemists working in academia, industry, and national labs. It is an unquestionable privilege to mentor undergraduate, doctoral student and postdoctoral co-workers, to support their development as scientists and onwards to career paths in and outside of academia.

I completed graduate studies at the University of Cambridge (UK), followed by postdoctoral stays at the Institute of Chemical Research of Catalonia (Spain), and at the University of California, Los Angeles. My independent academic career began at the University of Oxford before moving to Colorado State University, and has been recognized by the Silver Jubilee Prize from the Molecular Graphics and Modeling Society, the Harrison-Meldola Memorial Prize from the Royal Society of Chemistry, and the OpenEye Outstanding Junior Faculty Award from COMP. I co-authored a book of chemistry problems that has been widely distributed in UK high schools and I have served as head-mentor at the International Chemistry Olympiad.

I have participated in COMP meetings, having organized and chaired COMP symposia, and would be honored to serve division members as a Councilor. I am particularly interested in promoting the interactions between computational chemistry and other chemical disciplines and divisions, and in developing the ways in which our division serves an international membership.

❖ Qin Wu (Councilor Nominee)

I have been a staff scientist at the Center for Functional Nanomaterials in Brookhaven National Laboratory since 2008. My research primarily focuses on using density functional theory and other computational chemistry methods to study new materials with novel applications, such as organic electronic materials for photovoltaics, and doped 2D materials (graphene, MoS2, etc.) for electrocatalysis. I am also interested in using quantum calculations to generate reference data for force field development and collaborate with leading force field experts. Because CFN is a DOE Office of Science user facility, an important part of my job is to support external users' research by providing my expertise as well as resources at our high-performance computer cluster. Many of our users are experimentalists, from whom I have learned the importance of computations to their work. At CFN, we carry out and support computational researches not only on atomic-scale simulations, but also coarse-grained modeling, as well as data analytics and machine learning. It gives me a broad appreciation of computational approaches in chemical research.

Before joining BNL, I was a postdoc at MIT with Prof. Troy Van Voorhis where we developed a constrained DFT method to simulate charge transfer. I completed my Ph.D. at Duke University with Prof. Weitao Yang where I learned the fundamentals of density functional theory and worked on improving the exchange correlation potentials. I have been an ACS member for over 16 years. I was a co-organizer of the New York Theoretical and Computational Chemistry Conference (NYTaC3) from 2011-2016. I would be honored to represent the COMP division members as a Councilor. I am interested in enhancing interaction with other divisions and bringing exciting National Meeting programs to COMP members. I would appreciate the opportunity to learn from others' experiences and to contribute new ideas to the future success and health of our community.