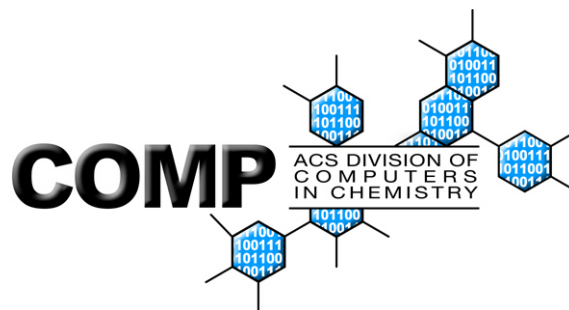


- Get involved with "COMP Division" via www.acscomp.org



COMP Newsletter

Statement from the Chair

Maria Nagan, COMP Chair 2018, reports on the division's status



Welcome Computers in Chemistry Professionals!

This year COMP has a number of projects underway. We are revising our website, figuring out tasks everyone can do to help out, recruiting more input from industry partners. COMP is also holding workshops for undergraduate students, providing special mentoring sessions for graduate student and post-doctoral women, putting on mentor lunches and holding our social for networking opportunities. If you have more activities you would like to see please get in touch with one of the executive committee members. We try to be as inclusive and open as possible.

Thanks for contributing to the COMP community,

Maria Nagan
Lecturer,
Stony Brook University
maria.nagan@stonybrook.edu

COMP Programming

We encourage everyone to start seriously thinking about the 257th ACS National Meeting (Orlando, FL March 31-April 4, 2019). The theme of this meeting is "Chemistry for New Frontiers". As part of this, COMP has put together another outstanding program!

The full meeting line up is listed below:

ACS COMP National Award Symposium:

- A ACS Award for Computers in Chemical & Pharmaceutical Research in Honor of Arnie Hagler (Invited)
- ACS Award for Research at an Undergraduate Institution: Symposium in Honor of Carol A. Parish (Invited)

ACS COMP "invited" Symposia:

- Computational Modeling in Two-Dimensional Materials & Heterostructures (Invited) (Engin Durgun, Tony Low, Ongun Ozelik)
- Drug Design in the 21st Century: Where Computational Methods Are & Are Not Useful (Invited) (Kevin Cusack, Michael Hoemann, Thomas Vargo)

- Electron-Molecule & Molecule-Molecule Interactions (Invited) (Revati Kumar, Jack Simons, Feng Wang)
- Machine Learning in Chemistry (Invited) (Christine Aikens, Adrian Roitberg, Sameer Varma)
- Sampling Conformations & Pathways in Biomolecular Systems: Recent Developments & Applications (Invited) (Ao Ma, Pratyush Tiwary, Wei Yang)
- Simulation of Protein-Membrane Interfaces (Invited) (Matthias Buck, Alemayehu Gorfe Abebe)

ACS COMP Contributed Symposia:

- Drug Design (Melissa Landon & Y. Jane Tseng)
- Molecular Mechanics (Jana Shen)
- Molecular Mechanics: Computational Studies of Transmembrane Proteins (Jana Shen)
- Molecular Mechanics: Recent Advances in Simulations of Nucleic Acids (Jana Shen)
- Probing Reactive Intermediates through Chemical Computations (Seonah Kim, Robert Paton, Shubham Vyas)
- Quantum Mechanics (A. Eugene DePrince III, Hrant Hratchian)
- Quantum Mechanics: Strong Electron Correlation (A. Eugene DePrince III, Hrant Hratchian)

- Material Science (Christine Aikens)
- Computational Studies of Water (Dan Sindhikara)
- Undergraduate Research Roundtable & Career Panel (Maria Nagan)

ACS COMP Posters:

- NVIDIA GPU Award (Mark Berger, Carlos Simmerling)
- OpenEye Outstanding Junior Faculty Award (Carlos Simmerling)
- Wiley Computers in Chemistry Outstanding Postdoc Award (Matteo Cavalleri, Carlos Simmerling)
- Chemical Computing Group Graduate Student Travel Awards (Karl Kirschner, Carlos Simmerling)
- COMP Poster Session (Henry Woodcock)

Please be aware of the deadline to submit abstracts to the **Orlando, FL National Meeting: Monday November 5th, 2018 at 11:59pm!!!** Full details can be found at the ACS website: <https://callforpapers.acs.org/orlando2019/COMP>

Finally, COMP would like to extend a special thanks to the individuals that dedicate so much of their time to putting together these outstanding National Meeting Programs!!!

- H. Lee Woodcock, PhD (Chair), University of South Florida
- Jana Shen, PhD (co-Chair), University of Maryland
- Christine Aikens, PhD, Kansas St. University
- A. Eugene DePrince III, PhD, Florida St. University
- Daniel Sindhikara, PhD, Schrödinger LLC
- Melissa Landon, PhD, Schrödinger LLC
- Terry Stouch, PhD, Science for Solutions
- Seonah Kim, PhD, National Renewable Energy Laboratory

- Robert Paton, PhD, Colorado State University
- Shubham Vyas, PhD, Colorado School of Mines
- Melissa Landon, PhD, Applied BioMath
- Yufeng Jane Tseng, PhD, National Taiwan University
- Maria Nagan, PhD, Stony Brook University
- Carlos Simmerling, PhD, Stony Brook University
- Karl Kirschner, PhD, Bonn-Rhein-Sieg University
- Hrant Hratchian, PhD, University of California, Merced
- Billy Miller, PhD, Truman State University

Undergraduate Programming

The annual COMP Undergraduate Workshop will be held at the Spring ACS meeting in Orlando. Undergraduate chemistry students will be selected for a series of undergraduate-focused talks. Two scientists (Prof. Donald Hamelberg, Georgia State University and Prof. Elena Jakubikova, North Carolina State University) will introduce students to molecular dynamics simulation methods and quantum calculations. Students will then present preview talks of their posters. The session finishes with a career panel that includes representatives from industry and academia. COMP has committed to running this workshop every Spring ACS meeting. So please send your undergraduate students. For more information, see the COMP website under "Recent News" or email: comp.ugworkshop@gmail.com

We will also be giving out Outstanding Undergraduate Research Awards in COMP at the Tuesday poster session as well as the Jeffry Madura Outstanding Undergraduate Research Award in the COMP subsection of the CHED Monday poster session.

COMP Awards

By: Carlos Simmerling,
Awards Coordinator.

The COMP Division is pleased to announce the winners of the COMP awards for the Fall 2019 National Meeting in Boston.

Chemical Computing Group Excellence Award for Graduate Students

The winners of the Chemical Computing Group Excellence Award for Graduate Students are: **Gabriel dos Passos Gomes** (Florida State University, Advisor Igor V. Alabugin), **Victor Fung** (U of California Riverside, De-en Jiang), **Rajat Maji** (Texas A&M University, Steven E Wheeler), **Qing Zhao** (Massachusetts Institute of Technology, Heather J. Kulik), **Hongyu Zhou** (Southern Methodist University, Peng Tao). The winners each receive \$1,150 in travel funds along with a 1-year license to CCG's MOE software.



The winner of the NVIDIA GPU Award for Best GPU Poster award will be announced after judging at the meeting. The winner receives an NVIDIA GTX Titan X card.



OpenEye Outstanding Junior Faculty Award Program

The winners of the OpenEye Outstanding Junior Faculty Award in Computational Chemistry are **Tim Kowalczyk** (Western Washington University), **Edward O'Brien** (Penn State University), **Amish Patel** (University of Pennsylvania), and **Diwakar Shukla** (University of Illinois at Urbana-Champaign). The winners each receive \$1,000.



Newsletter of the COMP division of the ACS
Fall 2018, Boston

Sponsored by OpenEye Scientific

Wiley Computers in Chemistry Outstanding Postdoc Award Program



Sponsored by John Wiley & Sons

The winners of the Wiley Computers in Chemistry Outstanding Postdoc Award are **Ka Un Lao** (Cornell University, Advisor Robert A. DiStasio Jr.) and **Josh Vermaas** (National Renewable Energy Laboratory, Michael Crowley). The winners each receive \$1,000 in travel funds along with a voucher for a free book from John Wiley & Sons, Inc. (up to \$250 value).

In addition to the awards listed above, the COMP division holds an annual Symposium on Emerging Technologies in Computational Chemistry at the American Chemical Society Fall National Meeting every year. Please apply to these awards in the future! Details of the award requirements and application procedures are provided at the Division's web site (www.acscomp.org).

The COMP Division expresses our sincere gratitude to our sponsors that make these awards possible, including the Chemical Computing Group, Wiley, OpenEye and NVIDIA.

Women in COMP

The Computers in Chemistry (COMP) Division of the American Chemical Society (ACS) believes in the potential of young women in Science and wants to foster their engagement in theoretical/computational chemistry.

With the aim of inspiring young women in pursuing their career as computational and theoretical chemists, COMP has organized the **"Women make COMP"** symposium at the **2019 Fall National Meeting in San Diego, California**. The symposium will include both graduate students and post-docs, while established

women PIs will share their research and career experience, such mentoring the next generation of women in computational chemistry. The symposium will include short oral presentations from the participants and plenary lectures from eminent women scientists from both academia and industry. This is a unique opportunity that COMP offers to help young women in recognizing themselves as computational and theoretical chemists, fostering their motivation in pursuing a career as a theoretician in academia or industry.

To apply, submit your abstract for the 258th ACS meeting in San Diego. The most compelling abstracts will be selected for an oral presentation and will receive the "Promise in COMP" award, which includes registration fees and a recognition plate. We will offer lunch, while an open discussion will be organized to give the opportunity to young women to receive outstanding mentorship.

For more information, send an email to the organisers: Giulia Palermo (gpalermo@engr.ucr.edu) or Maria Nagan (maria.nagan@stonybrook.edu). To apply, submit your abstract for the 258th ACS meeting in San Diego.

"Women make COMP" is funded by an Innovative Project Grant (IPG) of the American Chemical Society.

How can COMP reach you?

Updating your contact information.

You can check and change your email and mailing addresses on-line by logging in to the ACS home page and going to "edit my profile". You can also contact ACS Customer Service (1-800-333-9511 US or 614-447-3776 outside of US). The representatives from this department will be able to visually confirm whether your address has a "bad address" flag present.

COMP Social Networking

Connect with us! Choose your favorite social media channel and join the conversation. Our twitter feeds @ACSCOMP and @ACSCOMPprog spread the word about upcoming events at ACS meetings, major COMP programming, awards opportunities, and more. Join the ACS COMP group on LinkedIn and Facebook for COMP updates, job postings, conference news, and other major news in the COMP community. If you are interested in helping organize networking events in your local region, please email linkedin@acscomp.org.

COMP Secretary's Report

ACS returned their annual review of our division's report. We are pleased to report an overall healthy score, with solid financials, active programming, and popular member events like the Saturday social at ACS. They've heard our concerns about the distance and small space at recent national meetings.

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