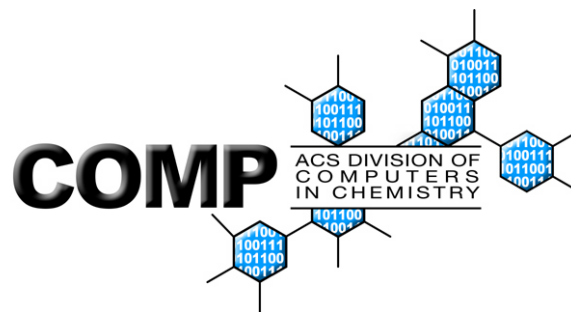


Spring 2018 Highlights

- Get involved with “COMP Division” via www.acscomp.org
- COMP Awards will be presented on Tuesday at the Poster Session



COMP Newsletter

Statement from the Chair

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



Welcome Computers in Chemistry Professionals!

The ACS Computers in Chemistry (COMP) Division continues to support its members through programming at national meetings, networking opportunities, outreach activities and awards. As we look to expand and support our membership, we would like to branch out to non-national meeting attendees. As such this year we will appoint ACS Regional Meeting Liasons, one for each regional meeting, to bring COMP programming closer to home.

Inclusive programming has always been valued in the COMP division. We usually are planning a year in advance. Prof. Luke Achenie (Virginia Tech) is our MPPG Liason. He is always keen to new ways to connect COMP to the main ACS program theme. If you would like to organize a symposium in COMP and/or related to the MPPG theme, please email the Program Chair Prof. Lee Woodcock (USF) to volunteer your services (lee.woodcock@gmail.com).

A new initiative to provide mentorship to female scientists in COMP kicked off with a post-doctoral mentorship breakfast in San Francisco with mentors Prof. Anastassia Alexandrova (UCLA), Prof. Zoe Coumia (Academy of Athens), Prof. Emily Carter (Princeton), Prof. Laura Gagliardi (UMN) and Prof. Nuria Lopez (IRB Barcelona). Women in COMP, spearheaded by post-doctoral fellow Dr. Giulia Palermo (UCSD), has now won an ACS Innovative Project Grant to expand these mentorship activities into a symposium (see Women in COMP section).

We continue with our COMP social on Saturday night, the Mentor Lunch, undergraduate workshop and awards. Is there a service you would like to provide to the COMP division? Or a networking activity you'd like to bring to fruition? Please email me with your ideas.

Thanks for contributing to the COMP community,

Maria Nagan
Professor of Chemistry,
Adelphi University
mnagan@adelphi.edu

The 253rd ACS National Meeting, (New Orleans, March 18-22, 2018), will showcase Nexus of Food, Energy & Water as the overall theme.

Overall, COMP programming is remaining a major part of the national meeting with over 600 papers expected to be presented in New Orleans. The full meeting line up is listed below:

ACS COMP National Award Symposium:

- ACS Award for Computers in Chemical and Pharmaceutical Research: Symposium in honor of Jürgen Bajorath

ACS COMP “invited” Symposia:

- Computational Catalyst Design for Energy Conversion & Storage (Christine Aikens, Cong Liu)
 - Structure-Based Drug Design for GPCRs (Ye Che, Veerabahu Shanmugasundaram)
 - Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation (Gerardo Cisneros, Peng Tao)
 - Insights into Structure, Function, Dynamics & Evolution of Enzymatic

COMP Programming

Mechanisms from Computational Simulation (Gerardo Cisneros, Peng Tao)

- Marriage of Machine Learning, Knowledge Representation & Chemical Sciences (David Koes, Edward Pyzer-Knapp)
- Large-Scale Applied Molecular Modeling (Raul Alvarez, Essam Metwally, Jose Duca, Juan Alvarez)

ACS COMP Contributed Symposia:

- Drug Design (Melissa Landon & Y. Jane Tseng)
- Molecular Mechanics (Michael Feig)
- Quantum Mechanics (A. Eugene DePrince III)
- Material Science (Christine Aikens)
- Computational Studies of Water (Dan Sindhikara)

We also encourage everyone to start seriously thinking about the 256th ACS National Meeting (Boston, MA August 19-23, 2018). The theme of this meeting is "Nanoscience, Nanotechnology & Beyond". As part of this, COMP has put together another outstanding program!

- Advancing RNA Designs (Christine Hajdin, Nicole Renaud, Bradley Sherborne)
- COMP Meets CRYO: New Frontiers in Flexible Fitting, Image Processing & Refinement of Cryo-EM Data (Michael Feig, Giulia Palermo)
- Computational Photocatalysis: Modeling of Photophysics & Photochemistry at Interfaces (Yulun Han, Dmitri Kilin)
- Data to Decisions: Frank Brown Memorial Symposium (Alexander Tropsha, Christopher Waller)
- Membrane Protein Simulations & Free Energy Approaches (Nilesh Banavali, Wonpil Im, Yun Luo)
- Molecular Mechanics: Computational Studies of Membranes & Transmembrane Channels & Transporters (Michael Feig & Jana Shen)
- Molecular Mechanics: Recent Advances in Carbohydrate Force Field

Development & Applications (Michael Feig & Jana Shen)

- Recent Advances in DFT & TDDFT: Theory & Simulations (Niranjan Govind, Chen Huang, Kenneth Lopata)
- Revolutionizing Chemistry with Artificial Intelligence (Payel Das, Rahul Das, Olexandr Isayev)
- Drug Design (Y. Jane Tseng & Melissa Landon)
- Molecular Mechanics (Michael Feig)
- Quantum Mechanics (A. Eugene DePrince III)
- Material Science (Christine Aikens)
- Computational Studies of Water (Daniel Sindhikara)

Please be aware of the deadline to submit abstracts to the **Boston, MA National Meeting: Monday March 26th, 2018 at 11:59pm!!!** Full details can be found at the ACS website:

<https://callforpapers.acs.org/boston2018/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
- Michael Feig, PhD (co-Chair), Michigan State University
- 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, Applied BioMath
- Yufeng Jane Tseng, PhD, National Taiwan University
- Maria Nagan, PhD, Adelphi University
- Carlos Simmerling, PhD, Stony Brook University

- Karl Kirschner, PhD, Bonn-Rhein-Sieg University

Undergraduate Programming

This will be the third spring meeting that we hold a workshop for undergraduate students. COMP sponsors the registration of 20-25 students. The workshop has two introductory talks covering quantum mechanical and molecular dynamics calculations. Then the students give pre-poster talks and it is wrapped up with a career panel.

Undergraduate Programming also covers Outstanding Undergraduate Poster Presentation awards. In both fall and spring meetings, we judge posters in the CHED-COMP and COMP poster sessions. Awards have been sponsored by the Council on Undergraduate Research, Wiley and COMP. In the CHED-COMP session, the award is named in honor of Prof. Jeffrey Madura (formerly Duquesne University). In total as many as 30 people volunteer to judge posters. If you would like to be on the list of judges, please email me (mnagan@adelphi.edu).

COMP Awards

By: Carlos Simmerling,
Awards Coordinator.

The COMP Division is pleased to announce the winners of the COMP awards for the Spring 2018 National Meeting in New Orleans.

Chemical Computing Group Excellence Award for Graduate Students

The winners of the Chemical Computing Group Excellence Award for Graduate Students are: **Stephanie Hare** (U of California Davis, Advisor D Tantillo), **John Karnes** (U of California Santa Cruz, I Benjamin), **Michiel Niesen** (Cal Tech, T Miller III), **Alice Walker** (U North Texas, A Cisneros), **Tzuhsiung Yang** (U Wisconsin-Madison, J. Berry). The winners each receive \$1,150 in travel funds along with a 1-year license to CCG's MOE software.

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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 **Heather Kulik** (Massachusetts Institute of Technology), **Daniel Lambrecht** (Pittsburgh), **Eric May** (Connecticut), and **Adam Willard** (Massachusetts Institute of Technology). The winners each receive \$1,000.



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 **Farnaz Alipour Shakib** (Rochester, Advisor Penfei (Frank) Huo) and **Feizhi Ding** (California Institute of Technology, Thomas F. Miller III). 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.

COMP Mentoring Luncheon

The American Chemical Society Computers in Chemistry (COMP) Division holds a regular luncheon for undergraduates and starting graduate students to ask questions about academic and industrial hiring processes. In the past, graduate students have found the most value in having a CV/resume review and discussing hiring with industry representatives that actively work with PhD's/post-docs. Undergraduates have found internships for post-baccalaureate training most helpful to discuss.

Previous industrial Mentors have been: Essam, Chris, and Veerabahu and Academic Mentors have been: Ajay, Shanadeen and others.

These are usually held at noon on Wed. of every meeting at a location close to the COMP programming. Check the website to find details on registering, there is about ten to twenty members at each luncheon so register to join the fun!



Women in COMP

The COMP division of the 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 in COMP" symposium at the 2019 Spring National Meeting in Orlando, Florida. The symposium will include both graduate students and post-docs, while established women PIs that 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 participate, send your CV, research abstract and motivation letter to Dr. Giulia Palermo (gpalermo@ucsd.edu). The most compelling abstracts will be selected for a short presentation, while all abstracts will be part of the COMP poster session.



How can COMP reach you?

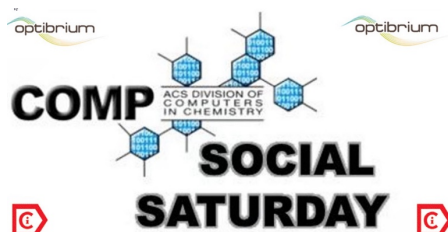
Updating your contact information.

You can check and change your email and mailing addresses on-line by logging in to the ACS home page and

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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



Stay connected with ACS COMP by joining us and >3000 members on LinkedIn or follow us on Twitter for the latest news @ACSCOMP. If you are interested in leading or joining a sub-group in LinkedIn to help organize networking events in your local region, please e-mail linkedin@acscomp.org.

The Computers in Chemistry Division invites you to attend the Spring National American Chemical Society 'COMP SOCIAL SATURDAY with CINF, sponsored by Optibrium', to be held at the Mardi Gras World Plaza in New Orleans from 7 p.m. until 9 p.m.

All COMP & CINF division members are welcome to attend, we ask that you register on [Eventbrite](https://www.eventbrite.com).

Currently, registration is being capped at 70 COMP/CINF members + 1 guest each.

Not a COMP member? Register at <http://web2011.acscomp.org/members/join-comp>

WHEN

Saturday, March 17, 2018 from 7:00 PM to 9:00 PM (Pacific)

WHERE

Mardi Gras World Plaza – 1380 Port of New Orleans Place, New Orleans.

(<http://www.rivercityvenues.com/venues/mardi-gras-world-plaza/>)

We look forward to seeing everyone soon!!

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