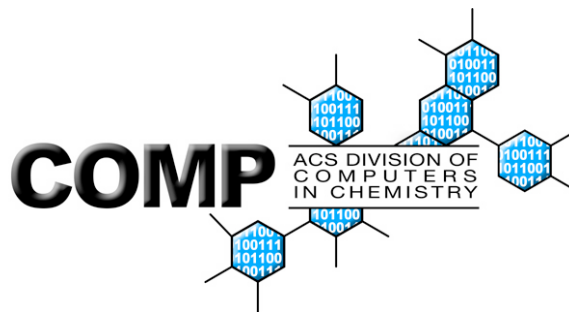


Spring 2017 Highlights

- 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

Chris Harwell, COMP Chair 2017, reports on the division's status

Welcome Computers in Chemistry Professionals!



Thank you for reading your Spring newsletter. I'd like to give a big shout out to all the volunteers that make Computers in Chemistry what it is. If you see one, please thank them for their efforts, which provide you with an opportunity to present and learn from scientific programming and network with your colleagues. If you have some time, please join them in shaping the future of Computers in Chemistry.

We are starting the Spring 2017 meeting in San Francisco off right with Computers in Chemistry social event on Saturday night - now even better with CINF, Cresset and Optibrium (see below for details). Thank you Lewis Whitehead for organizing this again! We are looking for an eager volunteer - maybe a knowledgeable local - to help organize a social event this fall in Washington D.C. Interested? Email me.

The programming for this meeting looks superb. There are really excellent symposia covering topics including drug

discovery, methods and material science. Some are particularly timely, like cloud computing and data science. Thank you Lee Woodcock and the whole programming team for a job well done!

Our annual planning conference was a big success. Thank you to the volunteers who gave up a weekend in February to review 2016 and plan 2017: we had twelve in attendance and several more on the phone. We do have challenges - like a decreasing financial allocation from the national organization and the ongoing struggle for good placement at national meetings - but we have a terrific team and it will be a fantastic year.

Thanks to the generosity of Slack for non-profits, we are piloting a new tool for communication and collaboration: <http://computersinchemistry.slack.com>. We have a limited number of spots available. Interested in helping us try it out? Send me the email address you use for ACS, we'll verify your membership and send you an email invite.

A big thanks to Carlos Simmerling for chairing the Awards Committee. The awards cover a wide range of categories - undergraduate and graduate students, as well as postdoctoral researchers, junior

faculty and career professionals. The Chemical Computing Group, NVIDIA, OpenEye Scientific Software, Schrodinger and Wiley help make these awards possible.

Finally, I'd like to ask you to personally encourage Computers in Chemistry membership and involvement. Being a member is about belonging to a diverse, open group of professionals. That membership supports our programming, awards and events. Ask a colleague if their membership is up to date. Encourage your co-authors and fellow presenters to join. Put a note in your email signature. Grab a sticker and display it proudly. We can't grow without you!

Chris Harwell, 2017 Chair
email: crharwell@yahoo.com
slack: @harwell

COMP Programming

The 253rd ACS National Meeting, (San Francisco, April 2-6), will showcase Materials Science as the overall theme. The role that computers and computational science plays in this area is particularly noteworthy. To this end, Prof. Christine Aikens has spearheaded the materials focused programming efforts in

COMP. Not only does this involve organizing the member contributed COMP talks in this area, but she also has recruited two member organized symposia in this area.

- Catalytic Materials from Molecular Insight (Bin Liu & Karoliina Honkala)
- State-of-the-Art Methods for Modeling Materials Chemistry (Ben Janesko & John Keith)

Overall, COMP programming is remaining a major part of the national meeting with over 600 papers expected to be presented in San Francisco. This is second only to the San Diego National Meeting where Computers in Chemistry was the national theme! The full meeting line up is listed below:

ACS COMP National Award Symposium:

- ACS Award for Computers in Chemical and Pharmaceutical Research: Yvonne Martin

ACS COMP "invited" Symposia:

- Computer-Aided Peptide Design (Qiaolin Deng & Sookhee Ha)
- Allosteric interactions and regulation of complex biomolecular systems: From proteins to cell signaling (Gennady M. Verkhivker & Chia-en A. Chang)
- Catalytic Materials from Molecular Insight (Bin Liu & Karoliina Honkala)
- Strong electron correlation and nonadiabatic dynamics (A. Eugene DePrince, III, Gergely Gidofalvi, & Edward G. Hohenstein)
- State-of-the-Art Methods for Modeling Materials Chemistry (Ben Janesko & John Keith)
- Data Science Challenges in Computational Chemistry (Michael Feig & Carlos Simmerling & George Vacek)
- Should I move my Computational Chemistry or Informatics

tools to the Cloud? (Essam Metwally & Veerabahu Shanmugasundaram & Jeff Blaney & Raul 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 254th ACS National Meeting (Washington, DC August 20-24, 2017). The theme of this meeting is "Chemistry's Impact on the Global Economy". As part of this, COMP has put together another outstanding program!

- Computational Design in the Vaccine and Biologics Therapeutic Space (Kerim Babaoglu & Melissa Landon)
- Modeling & Measuring Protein-Ligand Kinetics & Residence Times (Wendy Cornell & Joseph Morrone)
- Extending accuracy and scales with emerging computing architectures and algorithms (Gary Kedziora, Frances Hill, Yuri Alexseev, Paul Kent, Art Voter)
- Gradients, properties, and electron correlation, symposium in honor of Peter Pulay (So Hirata & Feng Wang)
- Molecular recognition: Revealing the effects associated with receptor-ligand binding (Emil Alexov & Ray Luo)
- Designing Chemical Libraries for Screening (Sourav Das & Anang Shelat)
- New Directions in Conformational Sampling Methods (Michael Feig & Jana Shen)
- Computational Studies of Membranes and Membrane-bound Systems (Jana Shen & Michael Feig)
- 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 **Washington, DC National Meeting: Monday April 10th at 11:59pm!!!** Full details can be found at the ACS website: <https://callforpapers.acs.org/dc2017/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

The second COMP Undergraduate Workshop will be held at the Spring ACS meeting in San Francisco. Undergraduate chemistry students (23) were selected for a series of undergraduate-focused talks.

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Two scientists (Prof. Eugene DePrince, Florida State and Prof. Carlos Simmerling, Stony Brook) will introduce students to quantum calculations and to molecular dynamics simulation methods. Students will then present preview talks of their posters. The session finishes with a career panel that includes representatives from industry and academia. Panelists this year are Dr. Woody Sherman (Chief Scientific Officer at Silicon Therapeutics and Adjunct Professor, UMass-Amherst), Dr. Kate Holloway (Principal Scientist, Gfree Bio), Dr. Carlos Simmerling (Professor, Stony Brook University) and Dr. Juan Santana (Asst. Professor, University of Puerto Rico). COMP has committed to running this workshop every Spring ACS meeting. So please send your undergraduate students. For more information, email: mailto:comp.ugworkshop@gmail.com

Council on Undergraduate Research and Wiley sponsored undergraduate poster awards in both the CHED section and the COMP poster session, respectively. Winners from the ACS in Philadelphia included Zachary Graziano (Mentor: Dr. Yu-Shan Lin, Tufts University), Jessica Niblo (Mentor: Dr. Robert Olsen, Stockton University), Lucas VanLaar (Mentor: Dr. Roger Dekock, Calvin College) and Edwin Fluck (Mentor: Dr. Vojislava Pophristic, University of the Sciences in Philadelphia).

COMP Awards

By: Carlos Simmerling, Awards Coordinator.

The COMP Division is pleased to announce the winners of the COMP awards for the Spring 2017 National Meeting in San Francisco.

Chemical Computing Group Excellence Award Recipients Announced

The winners of the Chemical Computing Group Excellence Award for Graduate Students are: **Fiona Kearns** (U South FL, Advisor L Woodcock), **Patrick Lestrangle** (U Washington, X Li), **Elvira Sayfutyarova**

(Princeton, G. Chan), **Kayla Sprenger** (U Washington, J Pfaendtner), **Mingzhen Zhang** (U Akron, J Zheng). 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 **Tom Kurtzman** (Lehman College), **Benjamin Levine** (Michigan State), **Marco De Vivo** (Istituto Italiano di Tecnologia), **Bryan Wong** (UC Riverside) and **Sapna Sarupria** (Clemson). The winners each receive \$1,000.



Wiley Computers in Chemistry Outstanding Postdoc Award Program

The winners of the Wiley Computers in Chemistry Outstanding Postdoc Award are **Makenzie Provorse** (UC Merced, Advisor C. Isborn) and **Varnavas Mouchlas** (UC San Diego, E. Dennis). 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).



Sponsored by John Wiley & Sons

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).

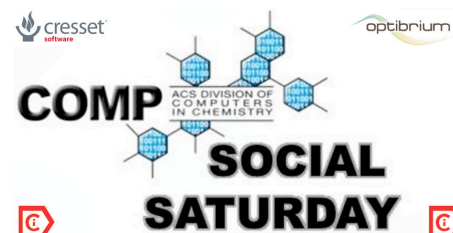
The COMP Division expresses our sincere gratitude to our sponsors that make these awards possible, including the Chemical Computing Group, Wiley, OpenEye and NVIDIA.

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



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 subgroup 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

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American Chemical Society 'COMP SOCIAL SATURDAY with CINF, sponsored by Cresset and Optibrium', to be held at Jillian's @ METREON from 7 p.m. until 9 p.m.

All COMP & CINF division members are welcome to attend, we ask that you register on Eventbrite.

<http://acscomp.eventbrite.com>

Currently, registration is being capped at 80 COMP/CINF members + 1 guest each.

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

WHEN

Saturday, April 1, 2017 from 7:00 PM to 9:00 PM (Pacific)

WHERE

Jillian's @ METREON - 175 Fourth Street, San Francisco, CA 94103.
(<https://www.jillianssf.com/contact>)

We look forward to seeing everyone soon!!

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