Women Make COMP

August 24, 2021
2021 ACS Fall Meeting – virtual

To inspire, motivate and support young women in computational and theoretical chemistry

Organizers

Giulia Palermo – University of California Riverside
Maria C. Nagan – Stony Brook University
Kira A. Armacost – GlaxoSmithKline

Description

Women are underrepresented in science, with a gender-gap particularly evident in physical sciences and technological fields. One way to address this, is to make sure that young women scientists at the graduate and post-doctoral level receive mentorship and encouragement to pursue future roles in academia and industry. The Computers in Chemistry (COMP) division of the American Chemical Society (ACS) wants to foster the engagement of these young scientists by making them feel that they belong in this vibrant community through the "Women Make COMP: Inspiring the Next Generation of Women in Computational Chemistry" symposium at the 2021 virtual Fall Meeting of the ACS.

This symposium will create an engaging and receptive environment in which established women principal investigators will share their research and career experiences with younger scientists, mentoring the next generation of women in our field. This unique opportunity will help young women in represent themselves in the computational chemistry community, fostering their motivation to pursue their careers as theoreticians in academia or industry. The call for proposals received more than eighty outstanding applications from young scientists. From these, five graduate students and post-doctoral fellows have been selected to give a talk, and ~30 applicants will present their research at the poster session.

The symposium will also include plenary lectures from respected women scientists representing established leaders and emerging young investigators in computational chemistry. These lecturers will share their experiences as women in science, while mentoring next generation professionals. The workshop will also create networking opportunities with established leaders working in industry, national laboratories, and government. This diverse pool of speakers representing different career stages and research environments will provide a broad perspective of professional opportunities for women scientists. Panel discussions in the afternoon session will create opportunities for graduate students, post-docs, and mentors to connect with one another on wide-ranging topics pertinent to women scientists.

Cover story: Ada Lovelace (1815–1852) was an English mathematician and writer, known for having founded computing science. She wrote the first computer program, disclosing for the first time that computers could do much more than just calculations. Her visionary perspective pioneered our current computer age. Painting by Giulia Palermo.

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Program

Morning session
Eastern Daylight Time (EST)

10:30 to 10:35 – *Introductory Remarks:* **Maria Nagan, Giulia Palermo, Kira A. Armacost, Dan Ortwine (Chair ACS COMP)**

10:35 to 11:00 – *Mentor Lecture:* **Laura Gagliardi** – University of Chicago

> Challenges and opportunities for women in theoretical and computational chemistry

11:00 to 11:15 – *Promise in COMP Talk:* **Angela Barragan** – University of Chicago

> Unveiling the reaction mechanism of covalent kinase inhibition by ibrutinib

11:15 to 11:40 – *Mentor Lecture:* **Neysa Nevins** – GlaxoSmithKline

> From academia to pharma: My 30 years journey in the COMP community

11:40 to 11:50 – *Intermission*

11:50 to 12:05 – *Promise in COMP Talk:* **Uchenna Anene** – University of Connecticut

> First-principles modeling of copper-epoxy resin interfaces for enhanced adhesion

12:05 to 12:30 – *Mentor Lecture:* **Rommie Amaro** – University of California San Diego

> SARS-CoV-2 through the computational microscope and the looking glass

12:30 to 14:00 – *Intermission*

Afternoon session

14:00 to 14:25 – *Mentor Lecture:* **Alice Walker** – Wayne State University

> Mentorship and outreach: Women working together in science

14:25 to 14:40 – *Promise in COMP Talk:* **Kayleigh Barlow** – University of Mississippi

> Anharmonic vibrational frequencies of isolated triatomic species: SCN^-, OCN^-, OCS, HCN, and HCP

14:40 to 14:55 – *Mentor Lecture:* **Solen Ekesan** – Rutgers University

14:55 to 15:20 – *Mentor Lecture:* **Heather Carlson** – University of Michigan

> Binding MOAD: Polypharmacology tools and drug repurposing

16:30 to 16:55 – *Mentor Lecture:* **Sharon Hammes-Schiffer** – Yale University

> Electron and proton transfer: Coupling together and to my career

16:55 to 17:10 – *Promise in COMP Talk:* **Anda Trifan** – University of Illinois

> Deep learning reveals wild-type and mutant Ras dimer interface formation in membranes

17:10 to 17:25 – *Promise in COMP Talk:* **Michelle Ernst** – Heidelberger Institute for Theoretical Studies

> Strength and nature of host-guest interactions in metal-organic frameworks from a quantum chemical perspective

17:25 to 18:25 – *Panel Discussion*

> Open discussion where participants and mentors will share their experience and career perspectives as a woman in computational chemistry.

18:25 to 18:30 – *Concluding Remarks*

Participant list

Organizers

Giulia Palermo	University of California Riverside
Maria C. Nagan	Stony Brook University
Kira A. Armacost	GlaxoSmithKline

Mentors

Laura Gagliardi	University of Chicago
Heather Carlson	University of Michigan
Sharon Hammes-Schiffer	Yale University
Alice Walker	Wayne State University
Neysa Nevins	GlaxoSmithKline
Rommie E. Amaro	University of California San Diego
Solen Ekesan	Rutgers University

Participants

Kayleigh Barlow	University of Mississippi
Anda Trifan	University of Illinois
Uchenna Anene	University of Connecticut
Angela Barragan	University of Chicago
Michelle Ernst	Heidelberger Institute for Theoretical Studies
Sanjana Srinivas	University of Delaware
Ariel Gale	Emory University
Christy Dyer	The University of Memphis College of Arts and Sciences
Sophia Hönig	Universität Hamburg
Mayar Mohamed	Southern Methodist University
Sara Tweedy	University of Michigan
Tingting Zhao	Southern Methodist University
Vyshnavi Vennelakanti	Massachusetts Institute of Technology
Tina Mihm	University of Iowa
Emily Landgreen	University of Iowa
Megan Simons	Southern Methodist University
Shree S. Santhanalakkshmi Vejaykummar	Colorado State University National Renewable Energy Laboratory, Golden, Colorado, United States
Narges Masoumi	Arizona State University
Amanda Sharp	Virginia Polytechnic Institute
Maya Petgrave	University of Waterloo
Katherine Oosterbaan	Lawrence Livermore National Lab
Andrea Bootsma	Pfizer Global Research
Miroslava Nedyalkova	Sofia University
Premila Samuel	University of Illinois
S. Maryamdokht Taimoory	University of Michigan
Caroline Kellogg	University of California San Diego
Stefania Monteleone	Evotec UK Ltd
Negin Forouzesh	California State University
Payal Chatterjee	University of Maryland
Emily Kempfer-Robertson	University of Louisville
Laia Delgado Callico	King's College London
Alice Romeo	Universita degli Studi di Roma Tor Vergata
Morgan Perkins	University of Mississippi
Carly Rock	University of Mississippi
Jacquelyn Mosely	University of Mississippi