

Women Make COMP: Mentoring the Next Generation of Women in Computational Chemistry

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ABSTRACT: The Women Make COMP symposium (258th American Chemical Society Meeting) aims at inspiring, motivating, and supporting young women in computational and theoretical chemistry. As a role model of the event, Ada Lovelace (1815–1852) was an English mathematician and writer, known for having founded computing science.



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 postdoctoral 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” symposium at the 258th Meeting of the ACS in San Diego. Ada Lovelace is the role model of the “Women MAKE COMP” symposium, **to inspire, motivate, and support young women in computational and theoretical chemistry.** 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.¹

“To inspire, motivate, and mentor young women in computational and theoretical chemistry”

The symposium has created an engaging and receptive environment in which established women principal investigators (PIs) shared their research and career experiences with younger scientists, effectively mentoring the next generation of women in our field. This unique opportunity has been offered to help young women in representing themselves in the

computational chemistry community, fostering their motivation to pursue their careers as theoreticians in academia or industry. Though this is the first such workshop aimed at mentoring young women studying theoretical and computational chemistry at an ACS conference, the call for proposals received more than 80 outstanding applications from young scientists. From these, eight graduate students have been selected for 15 min oral presentations, to be delivered to an audience of fellow students, postdoctoral researchers, and eminent women PIs at different stages of their careers. These talented young women scientists received the “Promise in COMP” award, which recognizes outstanding young talent with a waived registration fee for the conference and a recognition plate, kindly offered by the *ACS Journal of Chemical Information and Modeling*. The opportunity for a short oral presentation has also been to 30 other participants, who has showcased their exciting research.

The symposium has also included plenary lectures from respected women scientists representing established leaders and emerging young investigators in computational chemistry. These lecturers has shared their experiences as women in science and while mentoring next generation professionals. Prof. Angela Wilson (Michigan State University) will open the symposium. Dr. Antonella di Pizio (Technical University of Munich) and Dr. Eleonora Gianti (Temple University) will offer the perspective of women in the early stages of their careers. Prof. Anastassia Alexandrova (University of California Los Angeles), Prof. Carol Parish (University of Richmond),

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and Prof. Anna Krylov (University of Southern California) has also presented their research and shared their experiences as women researchers in academic settings. The workshop has also created networking opportunities with established leaders working in industry, national laboratories, and government. Among them, Dr. Debra Rolison (Naval Research Laboratory), recipient of the 2018 William H. Nichols Medal, will talk about important contributions of women in science. Prof. Monica Olvera de la Cruz (Northwestern University) concluded the symposium and conferred the eight Promise in COMP awards to outstanding recipients. This diverse pool of speakers representing different career stages and research environments provided a broad perspective of professional opportunities for women scientists. Round table discussions created opportunities for graduate students, postdocs, and mentors to connect with one another on wide-ranging topics pertinent to women scientists.

Over the years, the COMP division of the ACS has been very active in supporting research, mentorship, and networking of graduate students and postdoctoral fellows. This event was inspired by a session at the 2017 ACS meeting in San Francisco where Prof. Laura Gagliardi (University of Minnesota), Prof. Emily A. Carter (Princeton University), Prof. Anastassia Alexandrova (University of California Los Angeles), Prof. Zoe Cournia (Academy of Athens), and Prof. Nuria López (IRB, Barcelona) welcomed the planning of this symposium, actively participating in its organization and programming. This symposium received an Innovative Project Grant from the ACS, supporting the organization of the event and providing funding for the Promise in COMP awards. This commitment from the ACS recognizes the importance of inspiring and mentoring young women scientists in COMP-related careers in what will hopefully be the first of many symposia aimed at encouraging young women to pursue work in theoretical and computational chemistry.

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Notes

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