



## Calendar details

Date:	<b>Tuesday, 18 May 2021</b>
Time:	<b>9.00 am – 11.00 am (Melbourne Time)</b>
Event registration link:	<a href="https://www.eventbrite.com.au/e/australian-society-of-rheology-seminar-18-may-2021-registration-152039794117">https://www.eventbrite.com.au/e/australian-society-of-rheology-seminar-18-may-2021-registration-152039794117</a>

## Invited lecture

### **Professor Glenn H. Fredrickson**

(Departments of Chemical Engineering and Materials, Materials Research Laboratory,  
University of California, Santa Barbara, USA)

### **Presentation Title: Field-Theoretic Simulations of Polymers: Bridging Scales and Inverse Design**

Field-theoretic representations of many-body problems in classical and quantum statistical mechanics have been known for more than 50 years, but have largely enabled approximate analytical calculations. Over the past decade, my group has shown that complex-valued statistical field theory models of classical polymers can be directly tackled by numerical simulation. Such “field-theoretic simulations” (FTS) are advantaged over conventional particle-based computer simulations in a variety of situations, especially dense melts of high molecular weight polymers and systems with long-ranged interactions, such as polyelectrolytes. They are also well-suited for multi-scale simulations spanning nanometers to microns.

This talk will introduce the construction of field theory models of polymeric fluids and the FTS framework. Application examples to self-assembling polymers will be provided, along with a discussion of methods for bottom-up parameterization from all-atom force fields and inverse design.

## Speaker's biography



Glenn Fredrickson obtained his Ph.D. at Stanford University in 1984 and subsequently joined AT&T Bell Laboratories, where he was named Distinguished Member of the Technical Staff in 1989. In 1990 he moved to the University of California at Santa Barbara (UCSB), joining the faculties of the Chemical Engineering and Materials Departments. He served as Chair of Chemical Engineering from 1998 to 2001 and in 2001 founded the Mitsubishi Chemical Center for Advanced Materials (MC-CAM). Professor Fredrickson is currently a Distinguished Professor, holds the Mitsubishi Chemical Endowed Chair in Functional Materials, and serves as MC-CAM Director, and Director of UCSB's Complex Fluids Design Consortium. He has over 360 refereed publications, one book, and more than 15 patents in fundamental and applied

topics related to the statistical mechanics of soft materials, including polymers, colloids, and glasses. His



current research involves the development of statistical field theory based computer simulation techniques for the design of nanostructured soft materials.

Honors include the Polymer Physics Prize of the American Physical Society, the Cooperative Research Award in Polymer Science and Engineering of the American Chemical Society, the Alpha Chi Sigma and Walker Awards of the American Institute of Chemical Engineers, the Materials Theory Award of the Materials Research Society, the Collaboration Success Award of the Council for Chemical Research, and election to the American Academy of Arts & Sciences, the American Association for the Advancement of Science, and the National Academy of Engineering USA.

Professor Fredrickson has advised a broad range of companies in areas related to chemical and soft material science and technology. He has chaired Technical Advisory Boards for Dow Chemical, Mitsubishi Chemical, Apel Sciences, and Allergan Medical, and served on the Scientific Advisory Boards of Royal DSM, CSP Technologies, SABIC, SiO<sub>2</sub> Medical, and the green chemistry venture firms Segetis, Novomer, and Spero Renewables.

Since 2001, Professor Fredrickson has held various advisory and management positions with Mitsubishi Chemical Holdings Corporation (MCHC) and its subsidiaries. During the period 2001-2014, he was appointed as Corporate Science and Technology Advisor for Mitsubishi Chemical, Mitsubishi Rayon, and Mitsubishi Plastics. From 2009-2014, Professor Fredrickson served as Executive Director and Member of the Board of The KAITTEKI Institute, a long-term strategy unit of MCHC. During the period 2014-2017 he was appointed as Chief Technology Officer and Managing Corporate Executive Officer of the R&D Strategy Office of Mitsubishi Chemical Holdings. Since June 2014, he has been a member of MCHC's Board of Directors.

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