

Small Angle Scattering SIG Report 2021

SAS SIG Officers are:

- Steve Meisburger - Chair (Cornell University)
- Thomas Grant - Chair-elect (University at Buffalo)
- Sai Venkatesh Pingali - Secretary/Treasurer (Oak Ridge National Lab)

At the 2021 annual meeting of the ACA the SAS-SIG sponsored 1 workshop and sponsored or co-sponsored 5 half-day sessions:

Workshop:

- WK1: Characterization of Soft Materials Via Small Angle Scattering: Applications of Scattering for Polymer Systems

Sessions:

- 1.1.2 - Mapping Free Energy Landscapes of Molecular Machines (co-sponsored with Cryo-EM, BioMAC, YSIG, Light Sources)
- 2.1.1 - Evolving Enzymes (co-sponsored with YSIG)
- 2.2.4 - Membrane Protein Structure in Membrane and Membrane-mimic Environments
- 4.2.4 - Self Assembly in Soft Matter Systems
- 4.1.1 - BioWAXS: Experiment & Interpretation

In addition, one session was cancelled by the organizers (meeting costs for invited speakers were seen as prohibitive):

- Deciphering Chiral Structures in Soft Materials Via Correlative Approach of X-ray, Neutron Scattering, and Electron Microscopy

The sessions were well-attended. Approximate peak participation was noted for each as follows: "Mapping ..." (40), "Evolving Enzymes" (42), "Membrane ..." (23), "Self Assembly ..." (21), "BioWAXS ..." (49). While there were a few glitches due to the virtual format, the scheduled talks were a success, with robust Q&A and discussions at the end.

The Soft Matter workshop had about 14 people registered and there were between 6 and 9 attending the session across three days. Sessions were taught by Tyler Martin (NIST), Jan Ilavsky (APS), Greg Beaucage (U Cincinnati), Lucia Fernandez-Ballester (U Nebraska), and Tom Fitzgibbons (Dow).

SIG Meeting

The 2021 SIG Meeting, held virtually on July 26, 2021, was attended by between 18 and 20 people.

Session ideas for the 2022 meeting were collected by email before the SIG meeting and also put forward by members during the meeting. Sessions proposed at the meeting were further refined and prioritized through discussion with potential session chairs in the week between the SIG meeting and the planning meeting. There were 7 in total:

1. John Spence Memorial Session (suggested chairs: Richard Kirian)
2. Frontiers in SAS (suggested chairs: Jesse Hopkins, Max Watkins)
3. Phase separation and aggregation of bimolecular systems and intrinsically disordered proteins (suggested chairs: Richard Gillilan, Yun Liu)
4. Time-resolved SAXS/WAXS (suggested chairs: Tom Grant, Venky Pingali)
5. Hybrid Approaches to Understanding Macromolecular Structure (Suggested Chairs: Kushol Gupta, Dina Schneidman-Duhovny)
6. Scanning Imaging and Tomography Based on Scattering Contrast (suggested chairs: Lin Yang, Masa Fukuto)
7. Structure of semi-crystalline polymers as revealed through a combination of scattering and microscopy (suggested chairs: Tom Fitzgibbons)

A workshop on biological small-angle scattering was also proposed.

Nominations were solicited for the position of Chair-elect. Nominations were also solicited for Secretary/Treasurer as the two-year term terminates this year. Thomas Grant, Chair-elect for 2021, will serve as Chair for 2022.

Chair-elect Candidates:

- Durgesh Rai (XENOCs, durgesh.rai@xenocs.com)
- Suzette Pabit (Cornell, sap73@cornell.edu)

Secretary/Treasurer Candidates:

- Thomas Fitzgibbons (Dow, TCFitzgibbons@dow.com)

Planning meeting

During the 2022 planning meeting, sessions sponsored by the SAS were selected and/or combined with those of co-sponsoring SIGs. This resulted in 7 sessions with SAS as primary or co-sponsor:

- Day 1 AM - DeepMind/AlphaFold2 & RoseTTAFold: Use of the predicted Models in Structural Biology/Crystallography in the era of highly accurate models from sequences (BioMAC as primary sponsor. Suggested SAS chair: Dina Schneidman-Duhovny)
- Day 1 PM - Better Understanding Semicrystalline Polymers using complementary structure methods (co-sponsored with Industrial SIG, suggested SAS chair: Tom Fitzgibbons)
- Day 1 evening - John Spence Memorial Session (suggested chairs: Richard Kirian)
- Day 3 AM- Scanning Imaging and Tomography Based on Scattering Contrast (suggested chairs: Lin Yang, Masa Fukuto)
- Day 3 PM - Time-resolved Structural Dynamics (suggested chairs: Tom Grant, Venky Pinali)
- Day 4 AM - Frontiers in SAS (suggested chairs: Jesse Hopkins, Max Watkins)
- Day 4 PM - Phase separation and aggregation of bimolecular systems and intrinsically disordered proteins (suggested chairs: Richard Gillilan, Yun Liu)

It was decided to propose a workshop tentatively titled “Applications of Small Angle Scattering to Structural Biology: An Introduction”, to be organized by Michal Hammel (ALS).