



American Crystallographic Association  
August 2 - 7, 2020 #ACAgoesVirtual2020  
*TRAINING THE NEXT GENERATION*

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## 2020 Final Program

The scientific program features experts from all regions of the world (please note that all times are EDT). Click on the title for information regarding the session as well as the submitted abstracts. Sessions in the abstract system are listed as ending at 3:00 PM EDT however there will be approximately one hour at the end of the presentations for discussion.


Registered attendees will have access to the full schedule, list of abstracts and zoom links prior to the start of the conference.

[Program @ A Glance](#)

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Please note that this schedule is subject to change. Changes, if necessary, will be updated on this page.

### DAY 1: Sunday, August 2, 2020

<p>Sunday, August 2</p>	<p>12:00 PM - 4:00 PM EDT</p>	<p><a href="#">1.1.4 Microcrystal Electron Diffraction (MicroED) – Small Molecule &amp; Macromolecules</a></p>
	<p>Chair(s): <a href="#">Brandon Mercado</a> <a href="#">Tamir Gonen</a></p>	<p>The field of microcrystal electron diffraction has rapidly progressed over the past 6 years. Recent advances have placed microED at the forefront of structure determination. Several experimental protocols exist that describe the process of sequential sampling of diffraction patterns from nanometer-sized crystals while a sample is tilted in a transmission electron microscope. This session will be focused on advances in software/hardware and discussion of the results from microED experiments.</p>

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### Announcements



Sponsoring SIGs: Small Molecule/ Bio

Co-Sponsoring SIGs: CryoEM / YSIG

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Sunday, August 2

12:00 PM - 4:00 PM EDT

**1.2.5 From Materials to  
Crystallographic Analysis: A  
Neutrons/Materials/Powder  
Session**

Chair(s):

[Corey Thomson](#)

[Craig Bridges](#)

The Neutrons, Materials and Powder Diffraction SIGs are presenting a session that provides an opportunity to learn about materials ranging from correlated quantum materials to network structures, and new approaches to analyze crystallographic data.

Sponsoring SIGs: Neutron, Materials, Powder Diffraction

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Sunday, August 2	12:00 PM - 4:00 PM EDT	<a href="#">5.1.2 Hot Structures II</a>
	Chair(s): <a href="#">George Lountos</a> <a href="#">Nicole Fraser</a>	This session will be comprised of talks describing exciting new results in structural biology. The majority of talks will be selected from submitted abstracts.
Sunday, August 2	12:00 PM - 4:00 PM EDT	<a href="#">1.2.4 Advances in Fiber Diffraction and General Methods</a>
	Chair(s): <a href="#">Joseph Orgel</a> <a href="#">Tom Irving</a>	
Sunday, August 2	4:00 PM - 5:00 PM EDT	<a href="#">Poster Session I</a>
	Chair(s): <a href="#">Louise Dawe</a> <a href="#">Tiffany Kinnibrugh</a>	

## DAY 2: Monday, August 3, 2020

Monday, August 3	11:00 AM - 12:00 PM EDT	<a href="#">PL1 Etter Award: Nozomi Ando</a>
Monday, August 3	12:00 PM - 4:00 PM EDT	<a href="#">2.1.4 Frontiers in SAS</a>
	Chair(s): <a href="#">Tom Grant</a> <a href="#">Jesse Hopkins</a>	Recent advances in light sources, experimental methods and computational algorithms have enabled exciting new discoveries using small angle scattering (SAS). This session is devoted to discussing the latest advances in methods and applications of X-ray and neutron SAS. The primary aim is to bring together

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cutting-edge advances utilizing SAS on both soft matter and biological systems, including time-resolved studies, contrast matching, dynamic and flexible systems, hybrid modeling, novel experimental apparatus and methods, and new computational approaches. This session will reflect the state of the art in SAS methods.

Sponsoring SIGs: SAS  
Co-Sponsoring SIGs: Light Sources

**Monday, August 3**

**12:00 PM - 4:00 PM EDT**

**2.2.3 General Interest I**

Chair(s):

[Brandon Mercado](#)

[Marc Giulianotti](#)

[Kenneth Childers](#)

General Interest sessions are the forum for topics of broad interest to the crystallographic community or for presentations that do not fit the specific theme of other sessions. All presentations are selected from submitted abstracts.

Sponsoring SIGs: General Interest  
Co-Sponsoring SIGs: YSIG

**Monday, August 3**

**12:00 PM EDT - 4:00 PM EDT**

**1.2.1 Remote Access Facilities: What, Where & How?**

Chair(s):

[Eddie Snell](#)

[Jennifer Wierman](#)

Sponsoring SIGs: Light Sources/YSIG



**Monday, August 3**

**12:00 PM EDT - 4:00 PM EDT**

**2.1.2 Advances in Software Methods and Tools for Cryo-EM**

Chair(s):

[Xiaochen Bai](#)

[Zbyszek Otwinowsk](#)

Sponsoring SIGs: CryoEM

**Monday, August 3**

**4:00 PM EDT - 5:00 PM EDT**

**Poster Session II**

Chair(s):


[Louise Dawe](#)

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[Tiffany Kinnibrugh](#)

## DAY 3: Tuesday, August 4, 2020

<p>Tuesday, August 4</p>	<p>11:30 AM - 3:30 PM EDT</p>	<p><b><u>5.1.1 Structural Contributions to SARS-CoV2 and the COVID-19 Pandemic</u></b></p>
	<p>Chair(s):</p> <p><a href="#">George Lountos</a></p> <p><a href="#">David Rose</a></p>	<p>The Hot Structures session will feature talks selected from submitted abstracts describing the newest results from structural studies of biologically important macromolecules. Submissions are welcome that describe high-impact structures which provide insights into structure-function relationships, new biological insights and mechanisms, and methods development. Studies may include the use of X-ray crystallography, XFEL, hybrid methods, and cryo-electron microscopy..</p> <p>Sponsoring SIGs: BioMac Co-Sponsoring SIGs: YSIG, Canadian</p>
<p>Tuesday, August 4</p>	<p><del>3:00 PM - 4:00 PM EDT</del></p> <p><b>4:00 PM - 5:30 PM EDT</b></p>	<p><b>All Members Business Meeting</b></p>

## DAY 4: Wednesday, August 5, 2020

<p>Wednesday, August 5</p>	<p>11:00 AM - 12:00 PM EDT</p>	<p><b><u>PL2 Rognlie Award: James Holton</u></b></p>
<p>Wednesday, August 5</p>	<p>12:00 PM - 4:00 PM EDT</p>	<p><b><u>T1: Transaction: Structural Science: New Ways to Teach the Next</u></b></p>

 <p>#vACAmtg2020  Sponsor</p>  <p>#vACAmtg2020  Sponsor</p>	<p>Chair(s):</p> <p><a href="#">Joseph Tanski</a></p> <p><a href="#">Andrey Yakovenko</a></p> <p><a href="#">Christine Zardecki</a></p> <p><a href="#">Cassandra (Sandy) Eagle</a></p>	
<p><b>Wednesday, August 5</b></p>	<p><b>12:00 PM - 4:00 PM EDT</b></p>	<p><b><u><a href="#">4.1.2 Structural Dynamics I. Protein Collective Motions Studied by X-ray Scattering and Diffraction</a></u></b></p>
 <p>#vACAmtg2020  Sponsor</p>	<p>Chair(s):</p> <p><a href="#">Steve Meisburger</a></p> <p><a href="#">Doeke Hekstra</a></p>	<p>The macromolecules of life are often likened to elaborate machines, with many moving parts that must work collectively to achieve biological function. However, it has proven exceedingly difficult to understand how these machines work from traditional, static “snapshots” of structure alone. Thus, a new field of dynamic structural biology has emerged at the intersection of a diverse and evolving set of techniques. In Part I of this two-part session sponsored by Structural Dynamics, we focus on collective motions illuminated by X-ray scattering and diffraction. How are signals transduced within a protein? How are enzymatic activities coordinated in multi-step reactions? Are collective vibrational modes important for activity? This session highlights how cutting-edge X-ray methods, especially time-resolved SAXS/WAXS and crystallography, are providing insights into the dynamic nature of proteins.</p> <p>Sponsoring SIGs: SAS Co-Sponsoring SIGs: BioMac</p>
<p><b>Wednesday, August 5</b></p>	<p><b>12:00 PM - 4:00 PM EDT</b></p>	<p><b><u><a href="#">4.2.4 Physics and Chemistry of Matter Under Extreme Conditions</a></u></b></p>



Chair(s):

Yue Meng

[Bianca Haberl](#)

The application of extreme conditions such as pressure, temperature and field results in dramatic changes in all forms of matter. Under these conditions, matter undergoes phase transitions, displays rich new physical and chemical phenomena and can even yield new structures and materials not accessible in any other way. The aim of this session is thus to bring together the most recent advances and discoveries in both experimental and theoretical research that highlight these unique behaviors. Therefore, the session will address the many behaviors that are observed under extreme conditions. It will cover structural, electronic and magnetic properties, phonon and lattice dynamics, new materials synthesis, plastic deformation and melting. In addition, this session will also provide a forum for highlighting the state-of-the-art synchrotron and neutron techniques that enable new experimental research opportunities. Finally, it will also provide a platform for developmental ideas to expand the scope of future materials research under extreme conditions.

Sponsoring SIGs:  
Materials/Neutrons/Powder

Wednesday, August 5

12:00 PM - 4:00 PM EDT

**3.1.1 CryoEM in Pharma: Structure-based drug design beyond X-ray crystallography.**




Chair(s):

[Seungil Han](#)



[Alok Sharma](#)

For long, X-ray crystallography had been the backbone of structure based drug design. However, since the advent of direct electron detectors in 2012 and development in data processing algorithms in the field, single particle cryo-EM has become a widely and routinely used structure solution method for difficult targets including integral membrane proteins. Pharmaceutical companies kept them in par with the development of the technique and readily expanded their drug design portfolios to non-crystallizable proteins. In this session, we are going to learn about efforts and success with cryo-EM which pharmaceutical companies have made in the past few years. The session will also talk about challenges and path forward with this technique.

Sponsoring SIGs: Industrial  
Co-Sponsoring SIGs: CryoEM

Wednesday, August 5	4:00 PM EDT - 5:00 PM EDT	<a href="#">Poster Session III</a>
	Chair(s): <a href="#">Louise Dawe</a> <a href="#">Tiffany Kinnibrugh</a>	

## DAY 5: Thursday, August 6, 2020

Thursday, August 6	11:00 AM - 12:00 PM EDT	<a href="#">PL3 Patterson Award: Václav Petříček</a>
Thursday, August 6	12:00 PM - 4:00 PM EDT	<a href="#">T2: Transaction: Structural Science: New Ways to Teach the Next Generation (Part 2)</a>
 	Chair(s): <a href="#">Joseph Tanski</a> <a href="#">Andrey Yakovenko</a> <a href="#">Christine Zardecki</a> <a href="#">Cassandra (Sandy) Eagle</a>	
Thursday, August 6	12:00 PM - 4:00 PM EDT	<a href="#">4.2.2 Structural Dynamics II. Conformational Ensembles of Proteins Studied by Cryo-EM and X-ray Scattering</a>
		The macromolecules of life are often





Chair(s):  
[Liz Kellogg](#)  
[William Thomas](#)

likened to elaborate machines, with many moving parts that must work collectively to achieve biological function. However, it has proven exceedingly difficult to understand how these machines work from traditional, static “snapshots” of structure alone. Thus, a new field of dynamic structural biology has emerged at the intersection of a diverse and evolving set of techniques. In Part II of this two-part session sponsored by Structural Dynamics, we focus on the analysis of conformational and thermodynamic ensembles by cutting-edge approaches in cryo-electron microscopy (cryo-EM) and solution X-ray scattering. Recent developments in cryo-EM bring us closer to ensemble-like structural depictions that attempt to describe and better understand both compositional and conformational particle heterogeneity. Meanwhile, X-ray scattering allows for an unmatched view of a protein’s dynamic behavior in solution, and new avenues of analysis reveal meaningful structural information. This session highlights how cryo-EM and SAXS are uncovering the roles that conformational changes, intrinsic disorder, and structural variation play in protein function.

Sponsoring SIGs: CryoEM  
 Co-Sponsoring SIGs: SAS

<b>Thursday, August 6</b>	<b>12:00 PM - 4:00 PM EDT</b>	<b><u><a href="#">4.2.3 General Interest II</a></u></b>
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Chair(s):  
[Brandon Mercado](#)  
[Marc Giulianotti](#)  
[Kenneth Childers](#)

General Interest sessions are the forum for topics of broad interest to the crystallographic community or for presentations that do not fit the specific theme of other sessions. All presentations are selected from submitted abstracts.

Sponsoring SIGs: General Interest  
 Co-Sponsoring SIGs: YSIG

<b>Thursday, August 6</b>	<b>4:00 PM EDT - 5:00 PM EDT</b>	<b><u><a href="#">Poster Session IV</a></u></b>
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Chair(s):  
[Louise Dawe](#)  
[Tiffany Kinnibrugh](#)

## DAY 6: Friday, August 7, 2020

Friday, August 7	11:00 AM - 12:00 PM EDT	<a href="#"><u>PL4 Wood Award: Alan Alda Center</u></a>
Friday, August 7	12:00 PM - 1:00 PM EDT	<a href="#"><u>1.2.3 Communicating Science to the Public</u></a>
	<p>Chair(s):</p> <p><a href="#"><u>Brian Patrick</u></a></p> <p><a href="#"><u>Rajni Miglani Bhardwaj</u></a></p>	<p>Whether it be discussing climate change, public health policies, or simply conveying the impact of their research to the public, scientists need effective strategies to communicate and engage a broad audience. This session aims to bring together speakers discussing their experiences and approaches to scientific communication.</p> <p>Sponsoring SIGs: Communications Co-Sponsoring SIGs: Canadian</p>
Friday, August 7	12:00 PM - 4:00 PM EDT	<a href="#"><u>3.1.4 Cool Structures: Important Science from Small Molecules</u></a>
	<p>Chair(s):</p> <p><a href="#"><u>Louise Dawe</u></a></p> <p><a href="#"><u>Matthew Brown</u></a></p>	<p>This session aims to both highlight interesting structures of small molecules (&lt;100 atoms per molecule) and bring to the foreground the science enabled by small-molecule structure analysis. Speakers will be selected from contributed abstracts. Submissions from students are encouraged.</p> <p>Sponsoring SIGs: Small Molecule Co-Sponsoring SIGs: YSIG, Canadian</p>
Friday, August 7	12:00 PM - 4:00 PM EDT	<a href="#"><u>4.1.1 Methods and Tools for Crystallography and Cryo-EM Sample Preparation</u></a>
		With the technological advancements in



Chair(s):

[Eddie Pryor](#)

[Emiko Uchikawa](#)

both X-ray crystallography and Cryo-EM, structural biology techniques are becoming readily accessible to all labs. Although we are witnessing many significant strides in this field, the main bottleneck for both methods is still the preparation of high-quality protein samples. In this session we will highlight the latest methods and techniques for protein sample preparation for both crystallography and Cryo-EM experiments.

Sponsoring SIGs: Industrial, BioMac, CryoEM

Friday, August 7

12:00 PM - 4:00 PM EDT

**[3.2.3 Hot Structures I](#)**



Chair(s):

[George Lountos](#)

[Nicole Fraser](#)

This session will be comprised of talks describing exciting new results in structural biology. The majority of talks will be selected from submitted abstracts.



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