

## Small Molecule SIG Report 2017

The officers for the Small Molecule SIG for the 2017 calendar year are:

Chair: Stacey Smith (Brigham Young University)

Chair Elect: Graciela Diaz de Delgado (Universidad de los Andes Venezuela)

Secretary: Danielle Gray (University of Illinois, Urbana)

The Small Molecule SIG sponsored 5 sessions and co-sponsored 8 sessions at the 2017 meeting as follows:

- 1.1.3 Utilization of Small Molecule Crystallography in Pharmaceutical Development (co)
- 1.1.4 Engaging Undergraduates with Crystallographic Research (co)
- 1.2.4 Important Science from Small Molecules
- 2.1.4 NMR Crystallography
- 2.1.5 Cool Structures
- 2.2.2 Home-Built Software (co)
- 3.1.2 Mineralogical Crystallography
- 3.1.3 Using Standard Tools & Methods in Non-standard Ways (co)
- 3.2.3 Crystal Structure and Property Prediction (co)
- 3.2.5 Crystal Growth
- 3.3.2 Would You Publish This? (co)
- 4.1.2 Standard Practices in Crystallography III: Communicating Crystallographic Results
- 4.1.4 In situ and Operando Measurements (co)

These sessions were generally well attended.

39 members attended the SIG Meeting held on Monday, May 29, 2017 from 12:00 p.m – 1:25 p.m. The SIG discussed sponsoring 6 sessions and co-sponsoring 3 sessions at the 2018 meeting in Toronto as follows:

- Special Session in Honor of Richard E. Marsh (co-sponsor with Service SIG) – full day session
  - i. All agreed this session is a high priority
- Dynamic Crystals as Molecular Materials (sponsor) – full day session
- Crystallography at Extreme Conditions (sponsor) – ½ day session
- Crystallization on the International Space Station (co-sponsor with Service SIG) – ½ day
  - i. There was much discussion about this session. It was concluded that this session does not completely fit with the charge of the Small Molecule SIG, but that we are interested in seeing the session occur and would co-sponsor the session if it is brought forth by another SIG.
  - ii. It was additionally suggested that this session be broadened to include crystallography in conjunction with Mars missions.
- Crystallography in Synergy with Computation, Spectroscopy, and Synthesis (sponsor) – ½ day
- Would you Publish This? (co-sponsor)
  - i. It was suggested that this session be held in the evening on the day in which the Richard E. Marsh Session is run because these sessions would be complementary.
- NMR Crystallography – ½ day session
  - i. Manesh Mehta said that this session was well attended this year and that he would like to run it again next year. Additional co-sponsors are likely NMP and Canadian
  - ii. Lee Daniels just wanted to oppose something so he opposed this session.
- Mineralogical Crystallography – ½ day session

- i. Nicole Valdez felt that this year's session was well attended and that keeping a session like this as an annual session would encourage more members from the mineralogy field to come on a regular basis. Additional Sig members concurred with her opinion.
- ii. It was suggested that this session not be run concurrently with the session on Crystallography at Extreme Conditions because these sessions would compete for the same audience.
- Cool Structures – ½ day session
  - i. This is a yearly reoccurring session proposed by the SIG. Members put forth the yearly session in the meeting but no chairs were brought forth. Shao-Liang Zhang from Harvard agreed to chair the session after the meeting.

All sessions were voted on and approved by the SIG members unless otherwise noted. It was agreed that ranking all the sessions was not necessary because of the reasonable number of sessions that are proposed. Should the SIG need to sacrifice a session in the planning meeting, the full day session on Dynamic Crystals should be reduce to a ½ day session.

Other items discussed at the SIG meeting:

1. **H.D. Flack should be memorialized at the 2019 meeting** and the Small Molecule SIG should co-sponsor the session or possibly a transactions symposium.
2. **The name of the Small Molecule SIG should be changed to Chemical Crystallography or Chemical and Mineralogical Crystallography.**
  - Lee Daniels seconded the comment adding that from the commercial side they describe it as chemical crystallography, which allows them to broaden the scope and prevent misunderstandings.
  - Peter Mueller was in favor of the name change to be consistent with IUCr standards.
  - Christine Beavers and Nicole Valdez wanted the additional inclusion of Mineralogical into the name to broaden and clarify the scope of our SIG.
  - All members present were in favor of changing the name to Chemical and Mineralogical Crystallography. It was proposed that we start the process to change the name.
3. **The new early/formal proposal system elicited mixed reactions.**
  - Positive:**
    - It was an ok way to get everyone started thinking about future sessions.
    - It is a good way for those not able to attend the current year's meeting to propose a session for the following meeting.
  - Negative:**
    - The deadline was too soon. The original deadline was right in the middle of the semester and most members were preparing for this ACA meeting and didn't have time to think about the following year. It was also noted that many people realistically can't/don't think about next year's meeting and possible session ideas until they arrive at the meeting.
      - It was suggested that there be NO deadline for proposals prior to the SIG meeting.
    - The interplay of members at the meeting often leads to new ideas, and the new proposal system would not allow for that.
    - Sometimes it is necessary to see how the turnout is at the current meeting for certain sessions being run for the first time (such as the NMR session this year and Mineralogical session in previous years) before proposing that they be run again. The new proposal system would not allow for these 'trial runs'.
    - The extensive information required by the forms was a barrier for sessions being proposed, leading to the small number of session proposals submitted (3) prior to the announced deadline.

Members of the SIG agreed that a complete session's description including possible speakers was more work than likely necessary.

- It was suggested that a simplified proposal form including only the session title, proposed length, co-chairs names, and a 1-3 sentence description of the session would be more appropriate.
- The consensus was that both the advanced proposal system (with a simplified form and no deadline) and the prior method of proposing sessions in the SIG meetings would be beneficial and could be continued.

Possible Candidates for Chair Elect, 2018 are:

Christos Malliakas, Northwestern ([c-malliakas@northwestern.edu](mailto:c-malliakas@northwestern.edu))

Karah Knope, Georgetown ([kek44@georgetown.edu](mailto:kek44@georgetown.edu))

Possible Candidates for Secretary, 2018-2019 are:

Nichole Valdez, University of Idaho ([vald2292@vandals.uidaho.edu](mailto:vald2292@vandals.uidaho.edu))

Mike Takase, Caltech, ([mktakase@caltech.edu](mailto:mktakase@caltech.edu))

Respectfully submitted,  
Stacey Smith, Chair