

ACS Meeting San Francisco, CA Meeting Minutes March 21-25, 2010

COMP Programming Meeting 3/20/10

3PM-4PM

Kate, Hanneke, Emilio, Curt, Jeffry, Terry, Ed, Ralph, Scott Wildman, Jane Tseng

Thomas Strom representing History of Chemistry attended the planning meeting to discuss the Anaheim ACS meeting where that group will be organizing a session entitled Pioneers in Quantum Chemistry. The program will draw on COMP and PHYS and HIST. Not looking for funding, but looking for support from modeling software companies. Planning full day so 12 speakers, willing to expand if necessary. He would like an email sent to COMP members to solicit ideas for speakers, but COMP would prefer it go out in the newsletter or on the web.

Programming Report: Jeffry Madura

Current meeting is in good shape

286 talks

PHYS is not programmed next to COMP

A new symposium is called Recent Advances in Computational Chemistry series which is vendor organized represented by CCG, OpenEye BioSolvIt, Schrödinger.

Poster session is in a private room for about 100 posters

Boston meeting programming is underway, 18 symposia. As of March, there are 54 abstracts submitted, ACS deadline is the 22nd of March, COMP deadline is the 30th of March.

Terry Stouch will be putting together a session at an upcoming ACS meeting to discuss the recent advances in the PDB database

Action Item: At the Boston Meeting COMP needs to appoint an assistant program chair

COMP Executive Meeting 3/20/10

4-6PM

Present: Ed, Kate, Hanneke, Curt, Jeffry, Peter, Scott, Terry, Emilio, Jane, Carlos, Hamelberg, Sara Nichols, Chuck Reynolds, Luke

Agenda Item 1: Curt: Chair Report

Curt introduced the agenda and discussed the overlay of the meeting. A discussion began on the action items and the initial discussion of the procedures manual took place.

Action item: all procedure manual updates to be sent to Melissa once finished.

Concerning By-laws, Hanneke has looked over the bylaws, and many changes could be made. Asst Sec and Treasurer are not currently covered in Bylaws. One thing that has been done consistently different is nominations. Also different is the sending out of advanced copies of the abstracts for meetings which is not longer done since this information is now available online.

Action Item: for Sara to be added to the executive email list, Ed will look into this. Chuck would also like to be on the list (has a new email address).

Action item: Peter will coordinate review of bylaws with the ACS review process. Peter will determine how the bylaws have to be submitted. The bylaws committee will have to sign off on the bylaws, and then submit them in a final form.

Action item: All COMP committee members need to look over the bylaws and get back to Peter with feedback by April 17th.

Action Item: An email will be sent to the membership about voting for the bylaws, and this could happen in the 2010 or 2011 election. The vote on bylaws will not be with the election but will be sent out at a later date. This will be done by the assistant secretary via survey monkey.

Action Item: Ask Chris about the submission of the treasurer's portion of the annual report. Chris and Sara will look into getting this in by the deadline.

HP Junior Faculty Award may need to be renamed if the support does not continue to come from them. Chuck made the point that it would be hard to change the name unless they back out of sponsorship altogether. The naming of the symposium is more what the discussion was focused on, the symposia should be renamed HP Outstanding Junior Faculty Award.

The 2010 Nominations Committee is Hanneke, Kate, and Curt. Positions coming up for election are Secretary, Councilor, and Chair.

The ARCC contract review is underway, we are contractually obligated to purchase 2800 at 8 dollars a copy. They are in violation of contract by not distributing to us leaflets. We are locked into the April 5th renewal or it is automatic. We received a refund of \$2000 from Elsevier due to an error in the money they had been sending us for the last two years. Cost of a legal review of the contract has not yet been determined.

Kate has been looking through the COMP membership list and noticing that the membership does not include many peers, as is most likely the case for many division members. In other words, we need to all take a personal interest in recruiting into the division members we know personally.

Action Item: Look into how the email list can be distributed to the COMP exec committee if we would like to pursue a membership drive. This information may be in the disclaimer made available when rosters are downloaded. COMP members could send to Kate lists of people they know so that she can cross check the list for whom to recruit.

The paper archive is being sent to Jeffry from John Woolfrey

The question was raised as to whether we want to do more than financial help for regional meetings? This may include helping to organize, or making sure they have access to comp speakers. Would there be a specific benefit to COMP out of this collaboration? This was left as an open question, but may become more granular with the roll-out of COMP together.

Kate found a way via ACS which we can do teleconferencing if we would want to do a mid-meeting sometime in the summer. Terry mentioned that there may be other options for doing the same sort of thing for a set fee of ~\$50/month.

It was discussed again that COMP is the backup sponsor for the computers in chemistry award. This was voted on at the 2010 planning meeting and voted yes. Hanneke mentioned that we should be on top of the positioning of symposium into COMP programming.

Action Item: Hanneke will inform ACS that COMP will be the backup sponsor for the computers in chemistry award.

Agenda Item 2: Hanneke: Comp Together

Hanneke discussed the COMP-together initiative and mentioned that it will continue on, but was previously dependent on Allen having helped Hanneke with the web portion of the initiative. This will need to be prioritized along with the web work.

Agenda Item 3: Ed: Web Site

Web design: Ed has agreed to do web updating, and Curt wants to have this be a priority. Ed mentioned that he will need someone else to do this in the long run and that we need to identify a person to help out. Email distribution is a top priority. An advertisement could go out in a COMP email about looking for another person to do this web updating. Current sponsor list should be added to the web page.

Melissa Landon will be unable to do secretary next year.

Agenda Item 4: Ed/Melissa: Secretaries Report

Action Item: Ed will determine whether he is able to take on secretary full time or not.

Agenda Item 5: Sara/Chris: Treasurer's report

Financials are in good shape. The allocation and dues entries are increasing for COMP in 2009.

Agenda Item: Terry Stouch, would like to have money donated via JCMD; Springer. He would like this to be an automated function, in the budget pipeline/administrative pipeline. Terry and Jeff have been discussing possibilities:

- A) sponsor a regular symposium for instance Drug Discovery
- B) some type of award for industrial comp chemists
- C) have a separate symposium which is not one of the existing ones

Jeff motioned that we accept the money from Springer to support Drug Discovery, this was seconded by Curt and voted in favor of. Jeffry would like to keep open the possibility for an industrial focused award in the future.

Agenda Item 6: Awards Committee: Carlos Simmerling

Awards at San Francisco were well applied for, things look good. An email needs to be sent out about the upcoming awards. Carlos will send Melissa the awards procedures document to add to the e-archive. This will be the first year for the Graduate Award in Supercomputing. It might be good to add the requirements that you are required to be in the US and that you are a member of COMP for future applicants.

The ACS award for computers in chemistry needs some sponsorship input. We are paying for this ourselves in the meantime, but we need to look into other options.

Agenda Item 7: Programming, Jeffry

The vendor session is happening for the first time this year, and it will happen again in Boston. This symposium is listed under recent advances in computational methods.

Agenda Item: Ralph is working on alternative sponsors for ARCC. Elsevier publication of 2010 ARCC is underway and moving forward. Ralph will also pursue the creation of electronic versions of ARCC.

Agenda Item 8: Councilor Reports

Emilio: Meetings and Expositions. Organic does no programming on Thursday and this apparently has little effect on the hotel stays from Wed to Thurs as judged by previous meeting stats..

Peter: Nominations and Elections: No report.

Ralph: Committee on Science:

- 1) Initiative in alternative energy systems
- 2) Stem science technology engineering and math
- 3) 2011 international year of chemistry

Carlos: Constitution and Bylaws: nothing relevant to COMP.

Luke: MPPG: A flyer for thematic programming has been distributed. Luke discussed upcoming themes for future meetings. Would we ever want to pursue a combination poster/oral session where the presenters would give a talk, and then would have a poster in the same venue? This was left as an open question, but the committee liked the idea.

Curt mentioned we will be addressing ACS fellows nominations in the near future.

Submitted Ed Sherer, Assistant-Secretary COMP