

**ACS COMP Division Executive Committee Meeting**  
**March 21, 2009**  
**Salt Lake City, UT**

**Program committee meeting**

Present: Hanneke Jansen, Curt Brenneman, Jeffry Madura, Carlos Simmerling, Wendy Cornell, Chris Harwell, Emilio Esposito, Melissa Landon, Peter Jurs, John Woolfrey

Program Report: Jeffry

Recap of Philly meeting:

Good points: 13805 total attendees, 8600 registered, 3000 students, 1490 exhibitors (in middle between Boston and New Orleans)

Brief Discussion re COMP exhibitors: felt the situation in Philly was not optimal, also concerned that symposia are spread over the whole week. Idea: have symposiums last a couple days only without sessions overlap. Always try to have special symposia and awards early in the week. We get more \$\$ for Sunday and Thursday symposia.

Curt: Promisory Dewar endowment: 23-25k, we get 2500

Curt: don't have Thomas Kuhn paradigm shift at this meeting. Carlos - perhaps we should lower threshold so as not to intimidate people. Jeffry: need someone to proactively search the literature and invite speakers (Ant Nicholls?). Ant would like COMP to reconsider symposium times, and wants us to take a role in judging.

Washington submissions look pretty solid. 75-80 poster submissions, 30-35 for QC, 20-25 for MM, 8 talks for tools, visualization.

Curt: heard from Pharma people that SLC thin on industry-related sessions. General consensus is that more sessions will be relevant in DC. Emilio - should we have scripting/programming sessions at every meeting that focus on a set of tools easily accessible to chemists. Hanneke - always have good stuff in CINF, MEDI, and Bio. Emilio - need to communicate more with other divisions so as to avoid overlap in topics areas, etc.

Jeffry: audio and video from awards symposia from New Orleans is posted on website. Chris - should alert Patrick to notify Facebook and LinkedIn groups

This meeting: will be audio recorded again. Jeffry commissioned ACS to do this for \$350. We'll get a CD from them.

Curt: reminder of notice from ACS that if anyone is seen recording video, taking pics, etc. during symposium then someone should call security immediately. Carlos mentioned complaints from last poster session on taking pics of posters without permissions. Allowed to take pics of own posters, but need release form from ACS for taking pics of other posters.

Hanneke: we should record one session from each meeting. Emerging tech session in DC was suggested. Emilio also noted that the visualization and programming sessions will be recorded with slides.

Jeffry: in SLC: 225 papers, 58 posters. 5 are CCG, 4 are HP. Usually we're around 300. May be attributed to overall low attendance at this ACS.

Poster session on Tuesday. Plenty of food and beverage.

Washington meeting: still accepting late abstracts. Send to Emilio.

Wendy - should we record DC career symposium? Jeffry: Lisa is happy to do this and submitted abstract, which Jeffry will revise. Lisa will give 15 minute intro and guidelines, put up some questions, then split people up to talk. May be good idea to have panelists introduce themselves. Jeffry: can have Lisa put up slide with peoples pics and names to keep up for whole meeting. Wendy: current setup may lead to redundancies in questions asked. Jeffry will suggest to Lisa to add a couple extra speakers to speak on industry. Session is co-listed with CEPA.

Emilio: would COMP be interesting in "sponsoring" DC meeting symposia on Web MO? Workshop has been Emilio is going to get more info.

Hanneke:

Can we have a separate mailing list for people involved with programming? Allen will set up.

### **Executive committee meeting**

Present: Hanneke Jansen, Curt Brenneman, Jeffry Madura, Carlos Simmerling, Wendy Cornell, Chris Harwell, Emilio Esposito, Melissa Landon, Peter Jurs, Luke, Ralph Wheeler

Chair Report:

Communication and Outreach: Email exploder list is done, newsletter will be sent out today. Facebook group is fairly small, but Linkedin group growing steadily. New Linkedin features should facilitate communication with a larger community. Separate

jobs link might be useful.

Emilio: 1/2 of ACS members don't belong to a division - can we get in touch with these people?

COMP will still keep sending out stuff to CCL list. Jeffrey drafted a Wikipedia entry on ACS Comp.

Emilio: should send out notifier to other comp-related groups on linked in to make aware of our presence. Send out notice of sessions for DC conference to other groups (i.e. CCL) prior to registration for DC meeting.

Luke: Twitter?

COMP together: not much has happened yet. Allen is establishing website. Hanneke looked into Facebook, but doesn't seem easy to send group email. Action Item: Innovation grant proposal (Hanneke and Mel) - seed money for sponsorship, training organizers) next round is May 1st - could do training during SF meeting.

Travel policy: need to clarify who officers are (chair, secretary, treasurer, program chair?). Modified policy (2) to include other members of exec committee and appointed volunteers.

Peter: wording should be consistent among paragraphs (i.e change "covers" to "reimburses").

Carlos: should move discussion in paragraph 3 re deadline in paragraph 5

Peter: symposium organizers should clarify what is "reasonable"

Discussion ensued as to whether amount of reimbursement should be increased for officers. Peter: add separate paragraph that specifies additional funding may be available?

Newsletter is finished and sent out today. Orlando has created a flyer. Need a volunteer to print and distribute a flyer. Curt has volunteered to do it. Also need waiver forms printed. Carlos: session chairs should remind people of poster session/newsletter/flyer availability with refreshments in addition to recording policy. Carlos: print out

Hanneke: should develop PowerPoint show for DC meeting with general info on COMP membership (i.e. benefits, etc) to show before/between talks at sessions as well as during breaks. Mel volunteered to make presentation.

Elections: Jeffrey, Curt, and Hanneke comprise elections committee. Need to elect 2 councilors, 2 alternates, and chair. Assistant treasurer is also needed but it is an appointment position. The Asst Treasurer handles finances at local events, acts as liaison to sponsors, be direct link to people with sponsorship requests.

Wendy: newsletter looks good, no way to change.

Carlos: can we send out conference announcement on Tim Clark's birthday symposium.

Hanneke: prefer not to email, but put on website and LinkedIn group.

Secretaries Report:

Summary of motions:

via email: sponsorship of CERN for \$500 via email, policy statement on use of email list exploder

At retreat: appointment of Patrick and Melissa, motion not to have affiliated groups under same tax ID, voted on mailing of ARCC (reinstated and new members can receive copies as conditions allow, spend up to \$500 on networking software for COMP together.

Mel: membership numbers report.

Hanneke: do we want to do recognition of long-standing members? ACS recognizes 50 year members. Will people appreciate it? Since not much interest expressed, COMP will not.

Treasurer Report: Chris

The financial health of COMP is good.

Some un-cashed checks have been settled, but others are unknown. ~\$5k in uncashed checks.

major expenditures: retreat, meeting, and administration

sent out CERMACS money

have checks for poster award

needs to work on invoices and budget, but reimbursement and operational procedures are ok

division allocation should come within next week

Announcement: ACS symposium series in ebook format which can be archived by institutions. We and our editors get royalties for these.

Jeffry: summary of programming. Lisa has agreed to do career symposium in DC. She has already asked panelists (incl. Peter, Wendy, and Hanneke) to participate. Idea is to have two additional speakers from academia and industry as well as slide with pics of panelists and short bio.

SLC meeting: 225 papers, 58 total poster, 5 CCG, 4 HP. Lots of food!

Philly: 14k people, 1490 exhibitors, New Orleans ~1200 exhibitors, Boston ~ 1700 exhibitors. Exhibitors have different schedule for this meeting - are doing exhibits on Sunday from 6-830pm and a little longer on Wed.

DC meeting: about to wrap up. Have visualization and scripting sessions.

Next meeting in SF!

Emilio: looking for sponsors to cover registration fees for visualization and scripting session speakers. NVidia may cover visualization session, but need a sponsor for scripting. 8 speakers

Curt: ACS fellow nominations. This year we get to nominate 8 people, in future look at people whose science has been featured as well as service to division, etc. So far have ~20 people in mind, but need to narrow. Also need indicators of excellence (i.e. exec council, councilor, organized symposium. Primary person who nominates has to be an officer. Rest of letters should come from comp division officers. Curt, Jeffry, and Peter will head up nomination committee.

Wendy: update on JMGM. Editor stepped down. Wendy is heading up search committee (Hanneke, Peter, George, Jonathan Hurst). Wendy sent out full job description. CV, 3 letters of support, and a 2 page vision statement were requested. April 15th is deadline.

Carlos: awards

not a lot of submissions, couple last minute entries

9 applications for CCG (5 awarded)

7 or 8 for HP (4 awarded)

decisions have not yet been made

HP applicants are harder to get - sent email to CCL, CHARMM, Amber, Vmd

-should also send mail to established labs? new email list may help with recruitment.

Jeffry: may want to post on NSF REU program and conference, HBCU mailing list, also consider posting on Hispanic focused outlets.

-include on PowerPoint slide

-send email to PIs included on list of comp chem labs on website

- winners for this meeting are to be published in C&E news

28 page proceedings

- think about electronic archive
  - 2 tiered system for CCG awards: to encourage COMP membership, would get an increased amount. membership must be established prior to submitting application. "members get more." need to talk to Anna at CCG.
- Jeffry: what is main motivation for doing this? increase in comp membership will be minimal.
- decided to revisit once we have statistics from Carlos on membership status of past winners.
  - affiliate members? only if you are not eligible to become an ACS member or division is affiliated with another group.

idea: have a phone conference between spring and fall meetings to discuss issues?  
-Carlos will print certificates for HP winners

### **Councilor reports:**

Ralph: attended councilor's orientation. investigating committee options.

Carlos: assigned to committee on divisional activities, did not attend am meeting

Peter: nominations and elections. much of activities are secret. pub committee - 26 journals in acs, so handle journal evals and editor reappointments, etc. JCIM and JCTC are doing fine - not under evaluation or scrutiny. JCTC editorial office changes are being made to lessen Bill's load. JCIM went into monthly pub at beginning of year. JMC has been loathe to publish computational papers for a long time. Chief editor has been in his position for 40 years. Reappointments happen every 5 years. Committee is thinking of instilling term limits.

Emilio: meetings and expositions, sub committee for sites. up to spring 2019 - probably will be Orlando. 3 moneymaking sites are Boston, SF, and SD, so want to make sure that at least one meeting per year will be in one of those places.

Luke: attended meeting on themes for future ACS meetings. overall themes for meetings: spring 2009: challenges for the future, for dc: chemistry and global

SF: chemistry for a sustainable world Boston: chemistry for preventing and combating diseases chemistry and transportation (i.e. bioenergy).

group meets at every national meeting.

no discussion on location of symposia or sub-themes

Ralph ARCC: current volume has 11 contributions. has meeting here with Elsevier to

discuss size of print run and other issues. want to negotiate 2400 issues with options for extra. other is to get into libraries and university subscription as well as indexing individual chapters. as of now they are indexed in chem abstracts. alternative print formats - Allen talked to Elsevier and found out they are losing money, but Ralph was told otherwise. Ralph is going to look into it getting published by ACS books, which would get issues into libraries. Peter knows Ryan Crawford from pubs committee. will contact to introduce Ralph. \$\$ back from publishers regarding additional 400 copies charged for shipping that were not (2800 published, 2400 shipped).

ACS - moving to online proposal manuscript submission. available as both print and online.

Sponsor relations: Hanneke proposes phone conference with Anna and other four concerned sponsors if they would like to participate. In general need to be more communicative with sponsors. Assistant treasurer could help here as well as contacting prospective sponsors. We should let sponsors know how we acknowledge them.

Secretary John Woolfrey