

Minutes COMP Executive Meetings

Washington, D.C. August 15, 2009

Attendees: Hanneke Jansen, Jeffry Madura, Allen Richon (call in), Ralph Wheeler, Emilio Esposito, Carlos Simmerling, Sarah Nichols, Wendy Cornell, Adrian Roitberg, Curt Breneman, Patrick Lee, Rommie Amaro, Kate Holloway, Peter Jurs, Chris Harwell, Terry Stouch, Melissa Landon, Ed Sherer, Chuck Reynolds, Hendrick Heinz, Jane Tseuy, Dave Spellmeyer

COMP Executive Meeting

1) Recognition: Hanneke recognized Ralph and Wendy for outstanding service to COMP. She further recognized Wendy for contributions to the strategic planning process.

2) Six members of COMP were elected as ACS Fellows, they were Peter Jurs, Dave Spellmeyer, Michelle Francl, Ken Houk, Bill Jorgensen, and Greg Voth

3) A member of COMP can be nominated to sit on the Joint Board Council Committee, this COMP member must be a current or past officer or councilor.

4) Wendy mentioned that Jeffry has been selected as the next editor of JMGM.

5) Hanneke discussed the COMP together initiative under the agenda item Outreach and Communication. Currently, COMP has an innovative grant submitted to help fund the initiative. We will need web tools which aid in networking of organizers and attendees for successful local events. A discussion followed indicating that location may be an issue for holding events. It was suggested that academic institutions may be easier to gain access to compare with industry sites. A suggestion was made to add a section to the web page which identifies which meetings COMP members will be at. It was restated that local events will not necessarily be funded by COMP.

The committee voted to continue working on the COMP together initiative.

6) Jeffry gave a report dealing with programming at the Salt Lake and D.C. meetings. He mentioned exhibitors were way down in SLC and DC compared with previous meetings. Jeffry mentioned there will be a session celebrating Bill Jorgensen's contributions to the field at the Boston meeting. Peter suggested running the 'life after postdocing' symposium every meeting. Wendy requested that symposia titles be posted on the COMP or ACS web page as soon as possible prior to any given meeting.

7) Older volumes of ARCC 1-4 will continue to be used for recruiting. All old volumes now reside with Jeffry Madura.

8) Concerning outreach and LinkedIn, Patrick would like any members who are able to start topics on the discussion board to do so. He will also be pursuing a twitter account related to COMP.

9) The possibility of losing HP sponsorship money was brought up. This initiated a discussion on whether we might need to add a new COMP committee position titled 'fundraiser'. If anyone has ideas of sponsorship or award money, please contact Curt or Carlos.

10) Terry Stouch would like to sponsor some COMP function or award through his contact with the Journal of Computer Aided Molecular Design. The available money would be on the order of a few thousand dollars and could possibly go towards the set-up of an Industry focused award for COMP contributions to medicinal chemistry projects, etc.

11) The question was raised, and is still open, as to whether COMP should place links to sponsors on our site in addition to graphic logos.

12) For ARCC vol5, Ralph mentioned there are 8 sections ready. The galley proofs are ready for an October print run.

Hanneke: Outreach and Communication:

1. We applied for an innovation grant for CompTogether. This is for people who cannot attend meetings but want to be involved in COMP. Allen will create an online webtool to announce and allow registration events: seminars, mentor events, consulting events, lunches, etc.
2. We need a network of 'local champion's to send out invites to events and coordinate; have people for DC, Philly, SF, SD, and Boston areas.
3. Need to determine how to handle sponsorship. We need an asst treasurer! One idea is to have money go through COMP earmarked for events, although there is some concern over how funds will be earmarked. In absence of sponsorship, COMP does NOT have dedicated funds. Another idea: sponsor provide place and food, or else people meet up at bar or other gathering place and pay themselves.
4. Chuck commented on the increased difficulty in finding locations. Restaurants can be expensive, and harder to have speakers.
5. The innovative project grant is to support local champions and have a retreat to share experiences on logistical issues. Need to provide some guidance on how to handle sponsorship, etc.
6. Allen has started to put together registration form to gauge interest in certain events. Send email to list?
7. Emilio: should we hold meetings at academic institutions?
8. Kate: maybe have industrial and academic champion at each place? Have events at National Meetings? These special interest groups meet up to discuss ideas, get to know each other, etc.

9. Mel/Patrick: start sub groups on linkedin? Announce special interest meetings, who's going to conferences, etc.

10. If people are interested in certain subjects, should we email them only with those announcements?

Jeffry: Programming

1. Recap from SLC: 10550 attendees, ~3500 students, # exhibitors way down (783 vs usually 1100!). There were papers and posters, 166 oral presentations
2. In DC: 352 papers, 97 poster, 255 papers. Awards and posters on Tuesday. Symposia, emerging tech, leaving the nest on Monday - get scanner!
3. Two symposia will be audio and videotaped: emerging tech, molecular visualization
4. Peter: having leaving the nest symposium in SF if goes well at DC? Jeffry not opposed depending on interest in DC. May be good idea to do at every meeting for student attendees. We should also see how this affects mentor lunch attendance
5. There will be a symposia on Bill Jorgensen at the Boston meeting. Need ideas for topics, symposia. Boston will be Jeffry's last meeting as program chair; Emilio will take over
6. Wendy: put future symposia on website to plan ahead?

Hanneke: Recruiting

1. Use ARCC to recruit - Ed brought leftover vol 4. Everyone who signs up will receive one, and do three 3 drawings: 1 @ leaving the nest, 2 @ poster session. Will put flyer, signup sheets, and newsletter
2. Mel: will make ppt slides to put up at meetings

Patrick: Communication

1. 150 members on LinkedIn, 30 members on FB:
 - maybe LinkedIn is better to focus on.
 - get people to post interesting discussions? then can divide into subgroups
 - problem with companies posting to group? - can set preferences.
2. Allen: include copy of newsletter on LinkedIn and FB
3. Kate: use linkedin to advertise for COMPtogether?
4. Patrick: Set up twitter account so people could tweet at symposiums. Does this add value?

Patrick: people should set up twitter accounts and see how they like it.

Kate: get list of COMP attendees for national meetings and contact them about events happening during meeting.

Hanneke: keep email list to member benefits only - can post other things on CCL, LinkedIn, etc.

Web Report: Hanneke

- have password-protected area now on website
- we need more graphics!

- Wendy offered to organize highlights of ACS COMP fellows - Hanneke proposes to do one at a time?

-Ed: VMD and Pymol gave permission to use graphics from their websites

Kate: set up a competition? choose from images from meeting talks to highlight on website?

Sec Report:

Ed: 22% returns. Electronic elections helped! The more emails you send, the better

Mel: Member report. Maybe send emails to terminating members, survey to see why they left, reminder that they need to renew their membership - mine data to look at trends?

Treasurer's Report: Chris

- The financials are in good order.

- 2008 taxes completed

-Reminder to send reimbursement info, mail stuff to Chris's work or home address

Chris nominated Sara Nichols as asst. treasurer. Curt seconded. Unanimously voted in.

Carlos: Awards

We got about 2x as many applications as awards. need to advertise more, send out to membership, other email lists, etc. names of awardees will be in c&en news

SF mtg: uncertainty about HP - not in budget. OE offered to pick up. Change name to junior faculty award or have name associated with it? Carlos wants announcement out by end of this week.

Adrian: should we still do 2x/yr? Carlos thinks yes. If we don't hear from HP by end of week, then ask OE. Hanneke: Should mention Thomas Kuhn award in email re HP and CCG award.

Hanneke:ACS award for Computers in Chemical and Pharmaceutical Research - no sponsorship. ACS didn't tell us ahead of time. Need to have ACS notify us when sponsorship is up. Schrodinger sponsored for last 2 years, ACS will absorb cost for 2010 award, but we need a sponsor before October for 2011 award to happen. Chuck - does it need to be one sponsor? Yes, because it's a big deal.

Sponsorship

Hanneke: sponsorship money dwindling - should we bring in someone dedicated to fundraising?

Jeffry: keep a number of smaller awards in the division. Chuck: big award puts spotlight on COMP. Curt: if we keep HP, can we ask OE for \$10k for ACS award? May be worth more than Kuhn award. Chuck: even if we go in the red, support idea to contribute funds

Hanneke: propose to support 2011 ACS award for \$6400. Ralph seconded.
Unanimously approved.

Anyone with sponsorship ideas email Curt and Carlos.

Hanneke: don't have nominees for 2011, but have candidates from the last few years.

Terry Stouch: JCAMD sponsorship. Couples ideas: (1) sponsoring an award for industrial comp chem (2) sponsoring a recurring symposium. Wants to make it a recurring contribution; willing to entertain other ideas. Thinking about a ~\$15k contribution.

Peter: most helpful to division to make an agreement between journal and program chair to sponsor symposium 1 or 2x/yr. Can pick and choose what fits from meeting to meeting. Wendy: sponsor general drug discovery session. Jeffry and Terry can discuss what is appropriate for Boston mtg.

Curt: best paper award?

Jeffry: Nice to recognize industrial contributions, pick out best speaker and give them award.

Hanneke: like the idea of doing consistently every year instead of big awards.

Kate: tie award to articles appearing/to be in JCAMD?

Terry: wants to be a regular contribution and wants exposure to have JCAMD. Needs to have justification of exposure - i.e. letter detailing what contribution would get JCAMD.

Wendy: JCAMD award would go pretty far.

Jeffry: he and Terry will draft a document that will go to exec committee for final approval.

ARCC: Ralph: 8 chapters in four sections. galley proofs back, on schedule for Oct printing date, shipping date should be roughly the same. Elsevier okayed print run of 2400. Other issues: vol 4 shipping mistake - did not get money back. Ralph/Chris will follow up.

Chris: need to clarify how much we will pay.

Can we post articles on web? can post article titles and abstract in password protected manner

volume 6 will have 6 sections. March 1 2010 deadline for final manuscripts

major issues: 1. financial issue - back cover is up for bid again. Elsevier will let us sell ads on inside back pages, but need bids. 2. publishing company - do we want to go to other avenues of publication. Elsevier is pushing electronic publication. Also, need to penetrate into libraries. Elsevier not pushing to get ARCC in libraries. other ideas - ACS books? will talk to ACS books - may be able to get into ACS books package. We could also publish ourselves for cheaper. Are there advantages to be associated with major publisher?

chuck: electronic way to go. book/journal runs cutting way back.

Ralph will research acs books and report back.

Jeffry will get overrun copies and wrong address copies

Councilors and MPPG:

Luke: MPPG moved away from steering committee mode. Have 2010 and 2011

Spring 2011: Anaheim "chemistry of natural resources:
Fall 2011: "chemistry of earth, space, and water"
Spring 2012 "chemistry of life" - will focus away from health-related topics, i.e. evolution, etc
fall 2012 "chemistry of health"
themes for 2013 spring: energy fall: transportation (chemistry in motion)
Luke: would like to see more comp presence - will talk with Jeff and Emilio.

Carlos: divisional activities: subcommittee for constitution bylaws - nothing useful.
electronic meeting content delivery - ACS may have content provider? 60% of asked symposia agreed to recording. Summary on annual reports - we only have 3 negative tendencies (which is good!): leadership, bylaws.

Ralph: filled out paperwork for preferences for committee assignment. 2 competing votes. 1. Shorten timeline for national elections. 2. Changes to methodology whereby petition nominees now do not have to be vetted by council - that could be changed by petition. Some people think this is anti-democratic and a pull for power by nominations committee. Another petition has been set forth that would make that moot - cannot have a petition voted on that doesn't already exist. Everyone supports alternating presidency idea.

Peter: The pubs committee is making a big change. Individual members of society will not get print journals; electronic only starting in 2010. Too costly to continue. Can still get print version but won't get discount. Other big changes also going on due to loss of advertising revenue (down 40%) - people have been laid off.

Submitted Secretaries: Ed Sherer/John Woolfrey