

COMP Executive Committee Meeting
April 5, 2008
New Orleans , LA

Program Meeting

- 1) At the current meeting there are 9 joint symposia between ACS and AIChE
 - a. AIChE would like more joint sessions
 - b. Sessions are computational catalysis, phase equilibrium, computational evaluation of rate constants
- 2) General notes about current meeting
 - a. There are a few events co-sponsored with CINF
 - b. ACS award to Andy McCammon
- 3) Contribution statistics
 - a. Boston: 123 orals, 85 posters
 - b. New Orleans: 72 orals, 87 posters
 - c. Philly: 64 orals, 100 posters
- 4) Fall National meeting in Philadelphia will have symposia in: comp chem. and bioinformatics; QM/MM; comp approaches to fragment screening; free energy simulations; pharmacology/drug discovery; kinases; challenges in comp chem.; molecular mechanics forcefield development; CCG awards; HP scholars
- 5) Theme for Spring 09 conference in Salt Lake City will be nanoscience
- 6) Theme for Fall 09 Washington DC will be globalization of chemistry
- 7) The multidisciplinary program planning group (MPPG) which chooses themes for meetings has 5 full members (divisions with largest numbers of papers: total over last 4 meetings)
 - a. Organic, medicinal, polymers, colloids, and inorganic
 - b. 4 other divisions added by election
 - c. Jeffry would like us to have representation on committee
 - i. They can bring in high profile speakers due to large budget
- 8) It would be a good idea to start tracking submissions of papers and orals and identify those submitters which are not showing up to meetings.
- 9) There was discussion of the even programming rules: programs spread throughout week allow for COMP to receive more money annually.
- 10) Allocation algorithm gives more money for programs on Sunday and Thursday
- 11) There was discussion of whether to increase the allotted \$1000 for open bar at the poster session to \$1500, and this was agreed upon.
- 12) Jeffry is working on pod casts of some presentations. He would like to obtain PowerPoint presentations of talks, possibly with audio recording to post to the comp website.
- 13) A separate room for the comp poster session has been key for sequestering food and delivering awards. When this is not the case, food goes quickly to non-COMP members, and the awards are difficult to hear presented.

Executive Meeting

- 1) A paper agenda was distributed by Wendy
- 2) A paper summary of the budget was submitted by Curt
- 3) A paper summary of JMGM statistics was submitted by Andy
- 4) Wendy stated that we should continue to tighten up things we do well prior to taking on new ideas
- 5) Once the archive has been transferred to John, and scanned electronically we need to discuss how it will be backed up
- 6) Minutes from Boston fall 07 meeting need to be approved
 - a. **Action Item:** distribute minutes and vote [Ed]
- 7) Question was raised about whether membership in comp should be required for presenting a paper at the ACS meetings
 - a. Decided it is not possible to require, but that organizers should suggest membership in COMP for future submitters
- 8) Committee discussed elections and decided that policies should be readily at hand.
 - a. **Action Item:** when do elections happen, what is summary of what happens. [Ed, Hanneke]
- 9) Curt gave the treasurers report: see appendix
- 10) Wendy provided an update on ARCC in place of Ralph
 - a. The 4th volume will be published in November 08
 - b. Ralph is taking over for David
 - c. **Action Item:** rename sections of ARCC to remove ambiguous groupings [Ralph]
 - d. **Action Item:** devise system for section editors and contributors to be informed of deadlines in a timely manner, and of identification of section editors [Ralph]
- 11) Carlos reported on awards committee
 - a. 4 HP winners, 5 CCG winners
 - i. Would like CV submitted with application in future to make it easier to compare applicants
 - b. If applicants do not get award, they are transferred into appropriate talk/poster slot
 - c. **Action Item:** try and find ways to get more award applications
- 12) The newsletter was going to be ready prior to the New Orleans meeting for distribution on site, but this was slightly delayed. [Carlos, and anyone else with input]
 - a. Currently, COMP emails members twice a year with newsletter
 - b. **Action Item:** Orlando will email committee with the draft text of an email for approval, this text will indicate to COMP members we would like to begin sending them email for important COMP announcements. [Orlando]
 - i. The text/email will contain 3 links
 1. link to comp division website
 2. link to the newsletter

- 3. link to opt out of future emails from COMP via ACS.org
 - ii. motion was made by Peter to send email to all members
 - 1. sent to all members except those who had opted out
 - 2. motion seconded by Andy
 - 3. motion passed unanimously
- 13) an update on the website was given by Wendy on Allen's behalf
- a. question raised about whether to have Facebook presence for Comp
 - i. **Action Item:** create group; Michelle has created this group as of 4/08
 - ii. Discussion of adding a forum/chat room to web page so that COMP members could network and participate in discussion of COMP related topics
 - iii. Tie in the CCL job listings to the COMP website, it was decided not to reproduce this job listing, but link to it
 - iv. It is appealing to create the ability to network on the COMP website
 - v. Question was raised as to how talks (PowerPoint slides, audio, etc.?) will be placed on web site
 - 1. Will it be possible to password protect for COMP members only?
 - vi. Ed volunteered to help Allen with website and provide feedback
 - vii. **Action Item:** Michelle will research Computational Chemistry based educational web pages for creating a list of resources to include in an educational section of the COMP web page.
 - 1. Topics include: comp, phys chem., etc.
 - 2. [not being pursued at this time]
- 14) John was asked what the assistant secretary might do to spread out job load
- a. Possibility of handling the roster work
- 15) **Action Item:** procedural manual should be updated by all officers for their respective positions [all]
- 16) Peter gave the councilor's report
- a. From the Publications Committee
 - i. Bill Jorgensen was appointed editor of the same 2 journals for the next 5 years
 - ii. Open access issue arose again
 - 1. must send paper for open access if you have been given Federal funds: NIH support
 - 2. the paper must also be submitted to PubMed
 - b. From the Nominations/Elections Committee
 - i. Petition procedures are in flux; want to make it harder to get a nomination to the ballot for the national president position
 - ii. No run offs in the future, will have instant run off ballots
 - iii. The ACS would like to shorten time table of elections
- 17) Andy discussed work being done to revise division allocation formula
- a. Equation does not contain benefit for regional meeting work even though the ACS would like more of those types of interactions to take place

- 18) Wendy discussed some topics covered under Strategic Plan Goal 1 (Networking, Career Growth, and Outreach).
 - a. She mentioned the mentoring lunches were taking place on Monday at the New Orleans meeting.