

Spring 2011 ACS Meeting  
**COMP Committee Meetings**  
Anaheim, CA  
March 26, 2011

**Program Committee Meeting 3:00 - 4:00 PM**

In attendance:

Kate Holloway, Jeffry Madura, Emilio Esposito, Mel Landon, Ed Sherer, Veer Shanmugasundaram (tc), Ralph Wheeler

1) Denver Meeting Overview – Emilio

Program is shaping up and several non-standard symposia are in place.

If COMP fits in with theme for its programming, there tends to be more exposure for the division.

Eric Patterson will be overseeing the programming in quantum mechanics.

2) San Diego 2012

A symposium is being set up concerning polymers

3) Long-range planning ideas 2012 and beyond – Veer

Several symposia were discussed for possible inclusion in San Diego and Philadelphia.

**Executive Committee Meeting 4:00 - 6:00 PM**

In attendance:

Kate Holloway, Jeffry Madura, Emilio Esposito, Mel Landon, Ed Sherer, Veer Shanmugasundaram (tc), Ralph Wheeler, Sara Nichols, Peter Jurs, Rommie Amaro, Luke Achenie

Action Items

- 1) At least 1 month prior to Fall ACS meeting, Peter will draft an email and Jane will send out an email to the membership indicating that the bylaws have been changed.
- 2) Bylaws will be posted to website by Jane.
- 3) Web content needs to be updated by all
- 4) Ed will provide Jane with documents from COMP to post to web including minutes, bylaws, demographics, etc.
- 5) Ed to collate procedures manuals.

- 6) Election committee requested to send election ballot to Ed by May 1, 2011.
- 7) Request for any group receiving COMP funding is to have those groups supply a summary of the event within 1 month of event, to be sent back to the COMP secretary.

## **Agenda**

### 1) Chair Report, Kate Holloway

#### A) Review of Action Items from Retreat

- Bylaws revisions need to be distributed one month in advance prior to a regularly scheduled business meeting.

COMP members do not need to vote, just informed of the changes

The plan will be to not put the by laws into the 2011 election, instead send out bylaws to members 1 month prior to 2011 Fall meeting.

COMP exec committee will vote on bylaws at Fall 2011

- Thumb drive quote, Patrick Lee

1000 thumb drives at 1GB would be \$7

Some question about whether we should spend money on this since it is on the order of the amount of money we receive in dues.

We would like to see whether this is one quote or the best quote, and for now will table the discussion until the Fall.

Rommie mentioned that the memory sticks could be given as a gift to people who volunteer for COMP – mentor lunches or symposia organizers

### 2) Secretary Report, Ed Sherer

- Membership: the membership is slightly larger at 2250 as of 3/2011
- Election planning – all set on Survey Monkey, request for election ballot to be provided to Ed by May 1, 2011

### 3) Nominating Committee report: Kate Holloway, Curt Breneman, Jeffry Madura

- Election slate for 2011 – please send ideas for election slate as soon as possible to any member of the sub-committee

4) Treasurer Report, Sara Nichols

- Financial overview – financials are in good order

Curt will need to close Century CD fund

Receipts for reimbursement should be sent in by April 1. Maximum amount is \$2,068 per year.

5) Requests for COMP funding

- ACS Western Regional Meeting 2011 (Pasadena, Nov 10-12, 2011) - comp chem symposium organized by Ken Houk

- COMP will fund this event up to \$500

- "Chemistry By Design: Building at the Molecular Level" symposium at Denver meeting, organized by SMU grad students, co-sponsored by CHED

- [http://www.cendigital.org/cendigital/20110321\\_sub/?pg=56&pm=2&u1=friend&sub\\_id=vCqhbXUGX9mA](http://www.cendigital.org/cendigital/20110321_sub/?pg=56&pm=2&u1=friend&sub_id=vCqhbXUGX9mA)

- COMP will fund this event for \$500 if they have a significant component of COMP

6) Newsletter:

- there is significant interest in increasing the frequency of newsletters going out
- there is also a desire to have more up to date news articles posted to the web
- the frequency of newsletters could be helped with a rotating editor arrangement

7) Programming, Emilio Esposito

- Tuesday afternoon at Anaheim is a round table summarizing the Docking and Scoring sessions
- Denver program – deadline for submission of contributions is April 4, 2011
- see summary above
- many good symposia for Denver
- symposium concerning batteries is being organized by Bill Swope

8) Long-range programming, Veer Shanmugasundaram

- San Diego and beyond
- see summary above

9) Awards, Kate Holloway

- looking for ACS Fellows Nominations for 2011
- ACS Award for Computers in Chemical & Pharmaceutical Research
  - COMP suggested nominees?
  - sponsorship beyond 2012? Accelrys only funding until then

10) ARCC, Ralph Wheeler

- ARCC vol 7 coming together nicely, 14 contributions in 6 sections
- Elsevier printing around June
- still in need of advertising for the back cover
- PDF copies of previous versions of ARCC will not be provided except to authors

11) Reports from councilors & MPPG representative

- Ralph – Committee on Science and Awards Sub-committee
  - awards nominees have been selected for relevant awards
  - long range planning is being discussed in Committee on Science
    - national science concerns
    - should committee look at pioneers of science?
    - the committee is also looking to partner ACS members with business ideas with venture capitalist
- Peter – nominations and elections will meet Sunday and Monday
- Luke – theme for Anaheim is Chemistry of Natural Resources
  - theme for Denver is Chemistry of Air Space and Water
  - theme for San Diego 2012 is Chemistry of Life
  - theme for Philadelphia 2012 is Materials for Health and Medicine

12) Web site, Jane Tseng

- as an alternative to a Wiki, Jane's group can also use Google documents

13) COMP Together update, Jane Tseng, local champions

- Hanneke has put together a nice summary of a COMP together survey which she circulated to the committee

14) Innovative Project Grant proposals, all

[http://portal.acs.org/portal/acs/corg/content?nfpb=true&pageLabel=PP\\_TRANSITIONMAIN&node\\_id=1774&use\\_sec=false&sec\\_url\\_var=region1&\\_uuid=d59033a7-76a7-4096-9b87-92fdf5a437b4](http://portal.acs.org/portal/acs/corg/content?nfpb=true&pageLabel=PP_TRANSITIONMAIN&node_id=1774&use_sec=false&sec_url_var=region1&_uuid=d59033a7-76a7-4096-9b87-92fdf5a437b4)

- one idea is a grant for regional meeting awards: Jeffry and Carlos
- Hanneke has another idea for research revolving orphan diseases or neglected diseases – related to Open Source Drug Discovery : <http://www.osdd.net/>

Submitted: Ed Sherer - Secretary