

# COMP Division Programming Meeting

## Dallas, TX March 14, 2014

Present: Emilio Esposito, Jeffry Madura, Chris Harwell, Ed Sherer, Terry Stouch, Adrian Roitberg

- 1) San Francisco paper submissions are still open, will close on the 15<sup>th</sup>
- 2) PHYS at San Diego is running a symposium called the future of computational chemistry

### Agenda for Exec Meeting

Spring National Meeting

Dallas, Texas

15 March 2014

Fair Park 1 of the Omni Dallas Hotel.

3:00 PM

Program Committee Meeting

4:00 PM

Executive Committee Meeting

Welcome

Secretary Report – Ed Sherer

Treasurer Report – Chris Harwell / Sara Nichols

Programming Report – Emilio Esposito / Scott Wildman

CCG Awards – Petrina Kamy and Adrian

Councilors' Reports – Peter, Ralph, Melissa, Emilio.

ARCC – Ralph, Kennie

MPPG – Kennie and Terry substituting for Luke

Kennie re: 2016 San Diego Computers in Chemistry Theme

Outreach occurring this meeting:

Graduate and postdoc reception

Undergrad speed networking

Mentor lunches 'Short list' of members on which to draw for these events?

Should time allow:

Miscellaneous

Regional coordinator? Should we have one?

# COMP Division Executive Meeting

## Dallas, TX March 14, 2014

Present: Emilio Esposito, Jeffry Madura, Chris Harwell, Ed Sherer, Terry Stouch, Adrian Roitberg, Lorena Tribe (guest), Ralph Wheeler, Peter Jurs, Lee Woodcock, Petrina Kamyra (CCG), Melissa Landon

From planning retreat in Princeton (2/2014)

## ACTION ITEMS

- 1) **ACTION ITEM:** Emilio to update COMP web site mission statement to: "The Computers in Chemistry Division of the American Chemical Society promotes an interdisciplinary forum for those interested in developing and applying computational tools in the chemical, biological and materials sciences."
- 2) **ACTION ITEM:** COMP recommends to its councilors to vote against the change in allocation model at the Spring ACS meeting in Dallas **DONE**
- 3) **ACTION ITEM:** Ralph to work with Jeffry and Terry to identify options for alternative publishing of ARCC articles and end the current ARCC contract **DONE**
- 4) **ACTION ITEM:** Ed to update travel policy and post to website. "The Chair, Chair-Elect, Secretary, Asst Secretary, Treasurer, Asst Treasurer, Program Chair, and Program vice-Chair will be reimbursed by the Division for travel to each national meeting up to the cap set by ACS for travel reimbursement to councilors." Added in Dallas – member will perform duties they are attending meeting for (their position). Make a substantial contribution to the running of the COMP division effort at the national meeting. Request to include detail about how you will contribute.
- 5) **ACTION ITEM:** Kennie to send COMP sponsorship form letter (e.g., regional meetings) to Terry and Ed (as in requirements for having COMP fund the event); Chris and Sara to compare any other versions of letter to this letter from Kennie **DONE**
- 6) **ACTION ITEM:** Asst Secretary (Veer) will take on the responsibility of nominations and awards/grants for COMP. Chair and Secretary to forward relevant emails from ACS **DONE**
- 7) **ACTION ITEM:** Ralph will ask Curt Breneman if he wants to hold the position of fundraiser for COMP. If Curt is not interested, we will pursue other leads including possibly placing an advertisement on the COMP web page. **DONE**
- 8) **ACTION ITEM:** Mel will contact Schrodinger for funding possibilities (off line discussion needed for how much and what will money go for?)
- 9) **ACTION ITEM:** person identified as fundraiser should talk with Kennie Merz about his 2013 work
- 10) **ACTION ITEM:** Chair should send an annual email to membership which details what COMP does, and what links, etc are available: web, linkedin, etc.
- 11) **ACTION ITEM:** Adrian will look into the possibility of adding in a video series of COMP interviews detailing why people are in COMP and what they get out of it
- 12) **ACTION ITEM:** Ed to update COMP letterhead and send to Terry, Sara, Chris, etc. **DONE**
- 13) **ACTION ITEM:** Ed to request copies of all Chair, etc correspondence **DONE**
- 14) **ACTION ITEM:** Sara to make sure CCL is linked on COMP web page
- 15) **ACTION ITEM:** Sara to add links to all relevant blogs and forums for COMP content on the web page
- 16) **ACTION ITEM:** Emilio and Lee will develop a system of contacts for information gathering in a blog/wiki style resource on the COMP web page
- 17) **ACTION ITEM:** Lee to gather comments and provide a summary to Kennie capturing the comments from the group dealing with Kennie's request for identifying themes, organizers, possibly speakers, and the presidential session speaker (3-5 possibilities) for the COMP theme 2016. **DONE**
- 18) **ACTION ITEM:** Kennie to follow up with COMP to obtain summaries of his request for information related to COMP theme 2016. **DONE**
- 19) **ACTION ITEM:** Adrian will look into building a COMP website-hosted version of the list of minorities and women job seekers in COMP related fields
- 20) **ACTION ITEM:** Ed and Chris to complete annual reports by 2/15 **DONE**
- 21) **ACTION ITEM:** Kennie to proof and send for review the annual reports by 2/15 **DONE**
- 22) **ACTION ITEM:** Emilio completes programming section of annual report by 2/15 **DONE**
- 23) **ACTION ITEM:** Exec committee to vote on approval of minutes from Fall 2013 ACS meeting in Indianapolis while at Spring 2014 meeting **DONE**

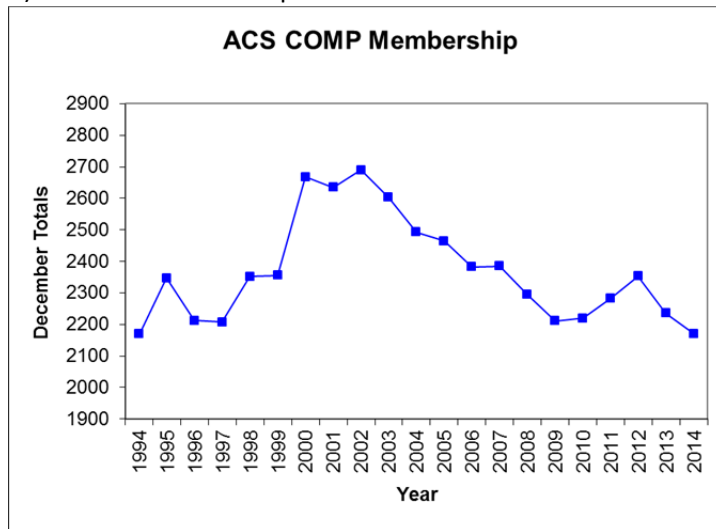
- 24) **ACTION ITEM:** From Indianapolis: Jeffry/Terry/Kennie will follow up with past winners of the Computers in Pharmaceutical Research for a discussion with ACS about continuing this national award
- 25) **ACTION ITEM:** Election committee begin work on 2014 election
- 26) **ACTION ITEM:** Emilio to investigate moving emailing of members from the current system to emailchimp
- 27) **ACTION ITEM:** Terry to contact ACS to have Award for Computers in Chemical and Pharmaceutical Research listed as being funded by COMP and not 'ACS'
- 28) **ACTION ITEM:** Terry to contact ACS concerning the selection committee for the national ACS award in computers in chemistry. Terry to contact Kate concerning details.
- 29) **ACTION ITEM:** Terry to gather nominations for ACS fellows 2014
- 30) **ACTION ITEM:** All Exec COMP members will bring a number of copies of the application to join COMP to place at relevant locations at the national meeting
- 31) **ACTION ITEM:** Ed to update list of COMP benefits on web page
- 32) **ACTION ITEM:** Adrian and Ed to run mentor lunches at Dallas meeting (to discuss with Rommie) **DONE**
- 33) **ACTION ITEM:** Ed/Lee/Adrian/Veer to put list of available COMP based speakers on the website. Pair it with a list of undergraduate focused groups in COMP.
- 34) **ACTION ITEM:** Scott to list the undergraduate poster award on the web site
- 35) **ACTION ITEM:** Scott to send out list of undergrad posters at Dallas meeting and help organize the awards for undergrad posters **DONE**
- 36) **ACTION ITEM:** Patrick to attend ACS 2014 Communications and Publications retreat
- 37) **ACTION ITEM:** Ed to post minutes from Fall 2013 ACS
- 38) **ACTION ITEM:** COMP to contact Chris and Laura about women in COMP
  
- 39) **ACTION ITEM:** Carlos, Terry, Kennie, and Adrian will post the guidelines for awards onto the website by San Francisco meeting
- 40) **ACTION ITEM:** Adrian and Peter will put together a scoring metric for the award judging

#### **Votes held at the Planning retreat:**

- 1) Motion by Adrian, Melissa seconded. Do not renew contract with Elsevier (& notify publisher of cancellation) and work with ACS or other journals to find an electronic publication option. Vote: 13 votes in favor, 3 abstentions (Interpretation – no longer publish print copies & lower cost)
- 2) Motion by Ralph, Terry seconded. Travel policy to be re-written: “The Chair, Chair-Elect, Secretary, Asst Secretary, Treasurer, Asst Treasurer, Program Chair, and Program vice-Chair will be reimbursed by the Division for travel to each national meeting up to the cap set by ACS for travel reimbursement to councilors.” Vote: 13 votes in favor, 1 abstentions
- 3) Motion by Ralph, Terry seconded. COMP continues to sponsor ACS national award for computers in chemical and pharmaceutical research and actively search for additional sponsors. Vote: 12 votes in favor, 0 abstentions

## Secretaries Report: Ed Sherer

### 1) Roster – membership decline



However the decline closely matches that of ACS membership as a whole and for a number of other divisions.

### 2) Election

A) The 2013 Election results are reflected in the 2014 current officers page

B) For 2014 we will be electing Chair for 2016, Councilor, Alt Councilor, and Secretary

### 3) 2013 Annual Report + Financial Report (via FORMS) completed and submitted

### 4) Electronic Archive: google docs – Ask Ed for access

### 5) Vote on acceptance of minutes from Fall 2013 meeting

A – vote in favor of posting minutes to COMP web

### 6) Action items and votes from the February Planning Meeting were discussed.

## Treasurer's Report – Chris Harwell

- 1) Division allocation came in and was a little less than last year, but not as much as two years ago
- 2) Division retreat was an all-time low amount, \$9K compared with \$16K for 2013 and \$21K of 2012.
- 3) The checking account had looked very low but Sara recently pursued some unpaid invoices and now its looking healthy.

- 4) Ralph noted that a new allocation formula was pending but, as below, he plans to vote against it as he is philosophically against it. It would mean a “few 100” dollars difference for us.

## **Programming Report – Emilio Esposito**

- 1) Dallas program looks very good
  - a. No sessions on Thursday
  - b. Lower number of sessions so not really possible to get to Thursday
  - c. Overall ACS attendance down for Dallas
  - d. Undergrad awards will be given out for undergraduate posters
  - e. We have some COMP undergrads submitting to COMP poster session and not the undergrad poster session. For this reason, we may need to rethink how we distribute the undergrad poster awards
  - f. Poster session refreshments cost \$10K (\$1000 for the bartenders), possibly less if not all drinks that are ordered are consumed.
- 2) San Francisco submission ends soon, but already have a large number
- 3) Boston is looking heavy in materials science
- 4) Interest is growing in San Diego. He plans for a Nobel symposium.

## **COMP Exec Award Criteria, Judging, and eligibility – Adrian Roitberg**

- 1) We need to establish a clear set of guidelines for how these awards are judged
- 2) We need to determine guidelines for applicants from the labs of Exec board members
- 3) Adrian sees a large correlation between the number of papers and winners
- 4) Jeff. M. would like to see judging criteria for the executive board and a policy for whether executive board students can apply.
- 5) Adrian: 20 of the 162 awards given in ?? time period went to students of EC members.
- 6) Judges for the OpenEye award were selected by Carlos from previous winners of the award.
- 7) Suggestions were made to put the criteria on the webpage. Also to blind the students' affiliations. And also to not list the number of papers per student.

ACTION ITEM: Carlos, Terry, Kennie, and Adrian will post the guidelines for awards onto the website by San Francisco meeting

ACTION ITEM: Adrian and Peter will put together a scoring metric for the award judging

This year COMP will do a 4/1 split of the 5 awards where 4 will go to comp related content in the undergrad section, and 1 will go to the COMP poster session.

Veer will help oversee award nominations at an ACS level, i.e., Kavli, ACS Fellows, Comp in Chem Pharm Sci., Chemluminary; Innovative Grants (IPG)

We have three volunteers to join in the undergrad speed networking exercise

We have representatives attending the graduate reception

We have 3 people doing mentorship lunches.

We will do a COMP Together happy hour in San Francisco.

## **Councilor Reports: Mel, Ralph, Lee, Peter, Emilio**

Mel attended the new councilor orientation.

Ralph attended the committee on science. He recommends we vote no to the proposed change in division allocation formula.

Emilio passes on the info that ACS is considering the removal of Thursday from the normal ACS schedule

All councilors will attend the council meeting on Wed, we will not need to send alternates.

## **ARCC – Ralph Wheeler**

- 1) Elsevier was surprised that we wanted to alter publication
- 2) Elsevier does own the name ARCC
- 3) Elsevier is willing to renegotiate the terms of the publication agreement
- 4) Ralph is continuing to work with Elsevier to revise if possible. More information should be available within a few days.
- 5) Recall notes about vote from above retreat discussion

**Curt has agreed to serve on COMP as the fundraiser . No plans have yet been discussed**

**Kennie gave an update on the Computers in Chemistry theme for 2016**

**Reimbursement travel policies, based on our recent decision to provide greater support, need to be determined. Reimbursement will be like that of the councilors. However, as minimum the EC member must fulfill their role's duties for that meeting and must attend the EC meeting. Further policy decisions are pending.**

Submitted

Ed Sherer (COMP Secretary)