# Minutes from the ACS COMP Executive Meetings
## San Diego, CA
## March 24, 2012

## Programming Meeting

Attendees: Sara Nichols, Jane Tseng, Michael Feig (MM session), Kennie Merz, Kate Holloway, Scott Wildman, Jeffry Madura, Ed Sherer

1) Larger number of papers compared to normal: 631 abstracts: 480 talks, remainder is posters
2) Philadelphia: programming is established and all standard symposia are present
   a. Abstract deadline is April 3
   b. COMP should co-sponsor with SOCED for undergraduate poster session
   c. For Philly and future, COMP will be a subdivision within undergrad session
   d. We would like ACS to allow for the undergrads to give the poster in both the undergraduate section and COMP
3) At Philly can we do a session on Sunday afternoon for undergraduates where we cover an overview of programming by COMP, and also have a way for undergraduates to present 2min(2 slides) on their poster. This would be followed by lunch with members of COMP and the wider community.
   a. Full first Sunday afternoon session
   b. **ACTION ITEM**: Reach out to undergraduates to let them know it exists
      i. Scott, Jane, Emilio, Jeffry, Jeff Evanseck
      ii. Letter is informative about content
      iii. Also invites them to give a 2 min presentation on poster
      iv. Will consider providing ARCC to all those who participate
      v. Will consider providing an award for best poster
4) Scott put together a list of all undergraduates with COMP related content, this list will be sent around to the Exec so that we can attend the poster sessions an discuss the posters with the presenters
5) It was discussed again whether COMP needs to be more restrictive on abstract submissions
   a. Is there a benefit to limiting the number of presentations per presenter/organization
   b. Suggestion was made to table the discussion until Emilio is around
      i. Possibly discuss at Philadelphia 2012

# Executive Meeting

Attendees: Sara Nichols, Jane Tseng, Michael Feig (MM session), Kennie Merz, Kate Holloway, Scott Wildman, Jeffry Madura, Ed Sherer, Rommie Amaro, Ralph Wheeler, Peter Jurs, Luke Achenie, Rigoberto Hernandez (PHYS councilor and DAC experience), Hanneke Jansen


1) **Welcome – Jeffry D. Madura**

    A) COMP would like to recognize Curt Breneman's efforts in identifying a replacement for the HP faculty award

    **ACTION ITEM** – Jeffry to send letter of thanks to Curt, and to OpenEye

    **ACTION ITEM**  Jeffry to organize- April 23 – deadline for nomination of ACS Fellows

    B) Peter has put together a description of the COMP annual retreats and will send the text to Jane for posting to the web

2) **Secretary Report - Ed Sherer**
    1) Election Results 2011
    a) COMP ran election for Chair, Treasurer, and Councilor
    b) Kennie Merz, Chris Harwell, and Ralph Wheeler were elected respectively
    c) Veer Shanmugasundaram was elected as Alternate Councilor
    d) offices and terms are as follows:

        Treasurer (2012-2015) Chris Harwell
        Secretary (2011-2014) Edward Sherer
        Councilor (2010-2012) Peter C Jurs
        Councilor (2010-2012) Carlos Simmerling
        Councilor (2011-2013) Emilio Xavier Esposito
        Councilor (2012-2014) Ralph Wheeler
        Alternate Councilor (2010-2012) Adrian Roitberg
        Alternate Councilor (2010-2012) Rommie Amaro
        Alternate Councilor (2011-2013) Patrick S Lee
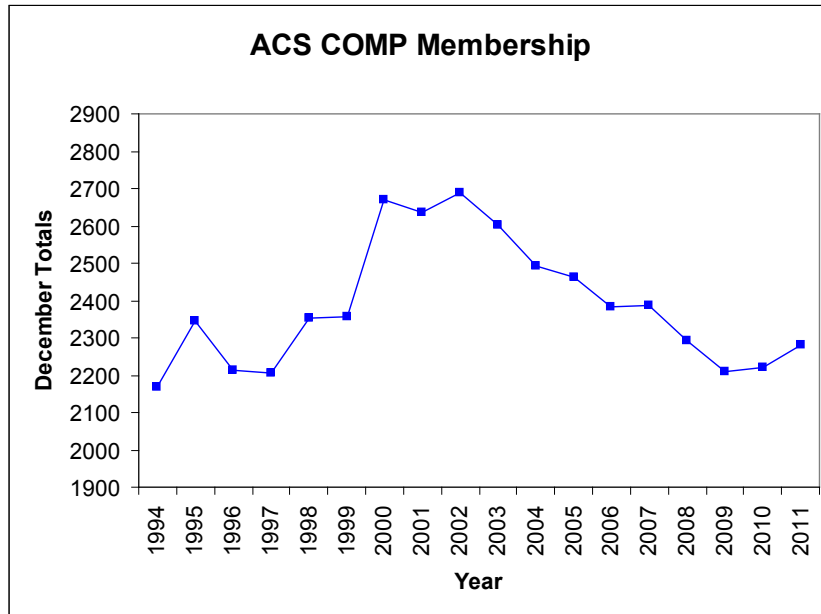        Alternate Councilor (2012-2014) Veer Shanmugasundaram

    e) Elections in 2012 will include: Chair, 2 Councilors and 2 Alternates
        1) nominations committee need to send in a list for the ballot by May 15
            a) **ACTION ITEM** – Jeffry and other chairs will be committee

2) Membership

**ACS COMP Membership**



3) Demographics Report:

As of 29 - Feb - 2012

**Member Type**

| Group | Count | % |
|---|---|---|
| Division Affiliate | 3 | 0.13 |
| Emeritus Member | 27 | 1.17 |
| Regular Member | 1,694 | 73.33 |
| Regular Student Member | 423 | 18.31 |
| Retired Member | 20 | 0.87 |
| Society Affiliate | 8 | 0.35 |
| Student Member - UnderGrad | 135 | 5.84 |
| **Total** | **2,310** | **100.00** |

**Industry**

| Group | Count | % |
|---|---|---|
| Academic Institution | 1,192 | 51.60 |
| Engineering/Construction Firm | 21 | 0.91 |
| Government | 133 | 5.76 |
| Hospital/Clinic | 19 | 0.82 |
| Independent Consulting | 98 | 4.24 |
| Independent Laboratory | 63 | 2.73 |
| Manufacturer - Industrial chemicals | 21 | 0.91 |
| Manufacturer - Other | 172 | 7.45 |
| Manufacturer - Petrochemical | 12 | 0.52 |
| Manufacturer - Pharmaceutical Co | 208 | 9.00 |
| Manufacturer-Agricultural | 2 | 0.09 |
| Manufacturer-Biotech/life sciences co | 45 | 1.95 |
| Manufacturer-Environmental/water | 2 | 0.09 |
| Manufacturer-Food/beverage/flavors | 6 | 0.26 |
| Public Utility/Transportation | 3 | 0.13 |
| Retail/Wholesale Trade | 22 | 0.95 |
| Other | 83 | 3.59 |
| No Response | 171 | 7.40 |
| N/A | 37 | 1.60 |
| Total | 2,310 | 100.00 |

4) Annual Report- submitted with Financial Report on February 15, 2012

5) Web page –
Send me your photos if you want them included on the Officers page

6) Review of Minutes will need to happen prior to posting to the web site.

7) Survey completed for the ARCC print vs electronic question

**1. How would you like to receive future issues of ARCC?**

| | Response Percent | Response Count |
|---|---|---|
| Bound paper copy | 19.9% | 79 |
| Electronic | 41.3% | 164 |
| Both | 32.5% | 129 |
| What is ARCC? | 6.3% | 25 |
| answered question | | 397 |
| skipped question | | 3 |

8) Veer will continue in the position of Asst Secretary and Alt Councilor

3) **Treasurer Report – Sara Nichols / Chris Harwell**
   Sponsorships
   HP Awards / CCG Awards
   1) The division allocation is 30% reduced from last year
   2) it seems that this is tied heavily to the attendance at the symposia
   3) **ACTION ITEM**: Sara will follow up with ACS and get back to the Exec about
      the allocation

4) Sara has put together a new letter which discusses the benefits of being a COMP sponsor

5) OpenEye will pick up the HP Junior Faculty Award in the place of HP
   a) award now renamed "OpenEye Junior Faculty Award
   b) in going forward, can the award be called: "The ACS COMP Junior Faculty Award sponsored by *InsertSponsorHere."?*

6) CCG looking to restructure their award, continuing for grad students, possibly expand to faculty, also consider themes
   a) we will need to discuss the expansion into faculty since we have a faculty award already
   b) CCG will attend the Philly meeting to discuss


## 4) Programming Report – Scott Wildman / Emilio Esposito
1) Newsletter is available for the meeting
2) talks up about 25-30%
3) April 3 = deadline for abstracts for Philly
4) Discussion of undergraduate symposia – see programming meeting notes above
   a) Exec committee is in favor of this


## 5) TDT – Hanneke Jansen
1) this initiative will be kicked off at the Sunday half day symposia (Hanneke, Wendy, Jane, Rommie)
   a) description and competition
   b) design workflows for one of 4 competitions
   c) datasets and judging panel is in place (available April, close Sept 5)
   d) winners are asked to submit a poster/presentation in NO, 2013
   e) https://sites.google.com/a/teach-discover-treat.org/web2012/


## 5.5) COMP funding for various initiatives
1) Should COMP fund multiple events for a single group
2) COMP will fund outside initiatives up to $500 per event (which support COMP's mission) and there will be no limit to the number of times a group can apply for funding, but each event will be decided on a case by case basis (as screened by Treasurer and Chair and forwarded to Exec for vote based on need).


## 6) Undergraduate Initiative – Kennie Merz / Jeffry Madura
1) Covered in detail above


## 7) Councilor's Report – Peter, Ralph, Emilio, and Carlos.
1) Peter has been elected to the Council Policy Committee
2) Peter's term on Nominations and Elections has ended
3) Ralph is sitting on Education Subcommittee
4) Rommie will be Alt Councilor for Carlos/Emilio
5) ACS is encouraging Alt Councilors to sit on Committees as well

**7.5) MPPG – multidisciplinary programming and planning group – Luke**
  1) theme this year is chemistry of life
  2) Luke is trying to support a computational aspect theme for a future meeting

**8) ARCC – Jeffry D. Madura – follow up in Philly**
  1) Jeffry spoke to JMGM about a special issue which would be ARCC
  2) Chris Harwell has also found an open source which could publisher
  3) discussed with Mike Frisch (considered the cost of ARCC currently is quite
   good)
  4) DOI and ISI are important considerations for alternative publishing
  5) a journal would be able to do color for articles
  6) ARCC - 0.72 impact factor for 2009

**ACTION ITEM**: Discuss publishing of ARCC

**ACTION ITEM**: Can Jane set up email for the executive officers which would be reflected to there email but would be something like COMP_program_chair@something.something.

Submitted: Ed Sherer, Secretary