

# COMP Minutes ACS National Meeting

Denver, CO

## Program Committee Meeting

3:15PM

Attendees: Emilio, Ralph, Jeffry, Scot, Hanneke, Eric, Veer, Curt, Melissa, Kate, Peter Jurs, Jane Tseng

- Anaheim Meeting COMP program was strong
  - Poster session was away
  - \$5000 – COMP pays for – Cash bar after that
  - Use all the food – Nothing goes to waste
  - Disney Hotel
- CINF welcome dinner
  - How much money ? How many people?
- Denver Meeting
  - 8000 registrants
  - Significant short fall
  - Allowing people to get registrations back
  - Couple of registrations pulled back
  - \$14,000 spend for food
  - Overall theme – Water (3.5 days), Battery, Drug Discovery programs, Material Science (3 days) – Get noticed/attraction
- Eric Patterson, Truman State – Organizing Quantum Chemistry Sessions
  - Quantum Monte-Carlo, DFT and couple of other sessions
- San Diego (huge meeting) San Diego Meeting – March 25-29, 2012
  - Middle of school year – Not much of impact
  - Abstracts: Last Monday 22<sup>nd</sup> August
  - Deadline: Nov 1<sup>st</sup>
  - Dates Set Out Further in Advance
  - Pushing it back gives organizers 7-10 days for pulling program together
- Thomas Kuhn Paradigm and Emerging Technologies
- Beta-Website (what's coming up)
  - Philadelphia
  - New Orleans
- Track number of attendees in a session
  - 1<sup>st</sup> talk – 100
  - 2<sup>nd</sup> talk – 10
  - File as 100
  - No of sessions, no of posters, no of people

- Double points for Sun-Thr
- ACS would like to have even programming
- 2 awards symposium – on always those days
  - ET – Sunday
  - Poster sessions – Tuesday evening
  - Wednesday – Anchoring session; Last big session
- 10 years out ACS meeting venues decided
  - # of rooms (whole hallway full of rooms)
- Spreading audience too thin with too many sessions vs making the program more diverse
  - Autocratic: Everyone
  - MEDI : General Session
    - Speakers don't feel welcome
- Philadelphia – Organizing
- Long Range Planning Committee to solicit proposals without picking a venue
  - No guarantees on venues
  - Use to fill gaps
  - Topic for Strategy COMP sessions
- Q:? Any request for career type workshops or symposium
  - Panel discussion +
  - Mentor Lunches – A day before that brown bag lunches + panel discussion
  - Put in the room (Monday over lunch)
  - Adjust COMP schedule to start at 2pm
  - Manipulate the schedule to accommodate to do it
  - Register for meeting – you pay for 10\$ -- do it that way
- Registration will open for Jan 15<sup>th</sup> –
  - Get menu for San Diego today from Jennifer
  - Cost issue
  - Is MEDI doing this at San Diego?

### **Executive Committee Meeting**

4:00PM

- Attendees: Emilio, Ralph, Jeffry, Scot, Hanneke, Eric, Veer, Curt, Melissa, Kate, Peter Jurs, Jane Tseng, Chuck Reynolds, Saurav Das

### **BYLAWS**

- Complicated process for making changes, how minor
- Did not vote on it at the last business meeting
- Present the new bylaws to the entire membership (amended)
- Sent out a brief email and asked people to comment

- Less than 5 comments
- Society was spelt wrong
- No hidden stuff in there – Take a vote on accept those amended bylaws
- Vote by all members – in a ballot (14)
- Vote by elected members – then vote
- Next Step : Peter to pass this on to the committee on constitution bylaws at ACS and then go from there – Follow through by email
- Curt went over Chris’s Treasurer Report
  - Curt to find out from Wally on CD check
  - Questions on some investment funds – Very conservative funds
  - Hard to get it out
  - Chris has provided a nice summary year split on early year dues and late year dues
  - Division Allocation – Income from National ACS high
  - Next Retreat – Las Vegas, NM
- Should also go into archives – Veer
- Pass on that – Current financial position
- New/Ongoing Funding – Merck has decided to give block grant to ACS as a whole
  - Bill Greenlee is handling all that
  - From pool Merck -- \$ to COMP
  - Vendors – How much they are actually contributing?
  - 2 funding request – Vote
    - Southwest regional Meeting \$1000 (8 votes)
    - Midwest Great Lakes Joint Regional Meeting \$600 (10 votes)
    - Raise the number and vote on a case by case basis
- Program
  - Anaheim – Great; Denver – Awesome; SanDiego – Huge
  - Eric Introductions
  - 50 people – boxed lunch at convention center – 20/person – 25
    - 2000 for 50 people
    - Sandwich, cookies, salad/fresh fruit, chips
  - Lunch ticketed through ACS – Panel Discussion/Mentoring Session
  - Action: Menu for SanDiego
  - Free WiFi at the Convention Center
  - PDF of onsite technical program
  - Beta-site for COMP – Upcoming symposia etc. – Accepted
    - Due dates for everything earlier – Nov 1<sup>st</sup> for San Diego Meeting
    - Organizers do not put abstracts in to the meeting
      - By ACS ID
  - Look back at programming and how many sessions/type of meetings/attendance
  - ACTION: Attendance sent to Program Chair – Get more data
  - Types: 1 ACS Award, Emerging Tech

- Contributed: Awards -- Location SF, Boston, SD,
- General:
- In addition that get our sponsors on how many people – Long Range planning on ET Sunday vs Wednesday – Give us some guidelines
- We might not have numbers for poster sessions
- Long Range -- P&G, Pfizer K'zoo, Lilly, EPA, Cincinatti, Chicago, IN schools
- Perspectives in Industrial CompChem – same thing with that
- Awards
  - ACS Fellows : 100% success – Tony, Hanneke, Jeffry , Andy, Curt
  - **Nominations for 2012**
    - **1<sup>st</sup> week in May**
  - 2012 ACS Award for Computers in Chemical & Pharmaceutical Research
    - Funding?
    - 300dpi or better quality – publication quality
    - Board with names of sponsors
    - Accelrys
    - Industrial People Get Nominated
    - Awards Selection Committee – Industrial People
    - 2 year commitment – 25K
  - A set of 4 HP junior faculty awardees
    - So far everyone will be here
  - CCG out of 5 one cannot make it
  - ET symposium – 1 contestant cannot make it
  - Program going along well
  - Keep these programs going with momentum
  - Get a hold of Carlos and publish a winner list
  - Commitment to the funders
  - Important to announce all winners and do electronic payments
  - One of us get home addresses to mail the checks
- Ralph Wheeler ARCC
  - Vol 7 has 11 chapters 5 sections
  - Galley proofs would be to authors
  - On track
  - Elseiever – No cost savings – 2300 copies instead of 2800 copies
  - Shipping savings is substantial – 11K
  - \$8 per copy to produce
  - **Ralph to aggressively explore alternative publishers**
  - **We should probably move electronic**
  - **ACS is moving strongly to electronic version – How interested would ACS be willing to do for us?**
  - **Timeline: We could do this by next year – April 1<sup>st</sup> deadline for Elsevier contract drop date**

- **Proof reading and formatting need to be done not camera ready**
- Self-publishing – Chris Harwell has suggested couple of options
- We do not have extensive penetration into library
- ARCC is abstracted and available in SCIFINDER and SCOPUS not ISI
- Elsevier contact changes once a year – Was going to contact someone in ISI – Does anyone have a contact at ISI – Serious concern for authors/potential authors
- Steve Myers – Office of international affairs
- Nancy Jackson
- Visa problems for speakers
- Advertising things internationally
- COMP division can be an international liaison for ACS
- Point of contact
  - Brazil – Ralph, Subash, Colombia – Indo US workshops
  - Have meetings outside the national meeting as well
- COMP together
  - 320 people signed up
  - 17 champions
  - TCs with each other
  - Career type events
  - 15min talks
  - SD, SF, CT
  - \$500 one time or once a year
  - Smaller groups -- \$200 can you use it up
  - Letter membership – for things to take advantage of
  - Sarah take on reimbursements for COMP together (offline)
  - Rommie was approached by Accelrys – San Diego to start an event -- Explore this a bit
  - Get people who are involved in the division
    - What are the opportunities for volunteers?
    - What sponsorships are available?
- Maybe do a Exec Comm Teleconf
- Website demo and beta session
- Everything has been copied – **Oct 1<sup>st</sup> deadline for release** – Keep updating this with new information
- Meeting minutes/agenda/technical program/content/image contest/awards
- Grant proposal submitted July 1<sup>st</sup> deadline
  - COMP TDT (teach-discover-treat) --
    - high quality tutorials for compchem
    - freely available software – opensource
    - tutorials will be made available thru website
      - drug discovery part
      - SD for half-day or full-day at NO

- Wrap up of competition – access to tutorials
  - How to go after a neglected disease target?
  - Wendy, Jane, Hanneke, Rommie
- \$7500 – support for two symposia and award for winners of competition
- Maybe you want multiple winners
  - Predicting what the target is
  - Predicting activity of targets
  - Characterizing ligands – label cpds as chelators, unstable
  - Overall winner based on best comp tool
- How to structure this competition
  - Will you get 5 submissions or 50 submissions?
  - Panel of judges/ahead – could be students/professor – see how this works
- Luke – San Diego – Fitting into Theme – Chemistry of Life
- Nominate a divisional 2012-2014 term – Committee of Science
- **Terry Stouch COMP nominee for committee of science**
  - Sci & Tech subcommittee
  - Education subcom
    - Science to Entrepreneurs
    - Venture capitalists
  - Public Policy
    - Insight, integrity, public policy
  - Awards SubComm
    - 1 nomin for ACS Fellow
  - Meetings and Acquisitions
    - 0.25M\$
    - Increase the meeting team
    - Registration shortfall
    - 7800 only – excluding reimbursements
    - Problems for society as a whole
  - ACS turns a profit on Boston, SF, SD
  - On site registration as an indicator for meeting success
  - 2012 – Meeting will increase to 360
  - Nominations & Elections (Jurs)
    - District Directors around the country
    - Put together slates for higher level committees
  - Publications Committees
    - Reviewing 3-4 journals with editors
    - Financially better year this year
    - Electronic publishing being discussed a lot
    - Iphone/Android app C&En news

- Ability to search ACS publications
- Subscribe to specific journal or packages across the journals
- 2 new journals – ACS Synthetic Biology, MacroLetters
- Publication process more efficient
- Concerns about plagiarism
- More and more automatic tools being put in place
- Feeling a lot of pressure from open-access side
- Wellcome Trust and Howard Hughes Foundation are discussing funding journals that are free.

Submitted: Veer Shanmugasundaram – Asst Secretary