Fall ACS Meeting
COMP Programming Meeting August 18, 2012
Philadelphia, PA

3:00-4:00PM

Attendees
Emilio Esposito, Ed Sherer, Jeffry Madura, Orlando Acevedo, Kennie Merz, Kate Holloway, Jane Tseng, Ralph Wheeler, Wendy Cornell

Programming Meeting

1) 2013 meetings are in New Orleans and Indianapolis in Spring and Fall, respectively.

2) We need to make sure that during symposia, an accurate and maximum number of attendees are noted as this influences our annual allocation.

3) Possibilities for increasing turnout, or concentrating attendance
- a. only 5 invited symposia
- b. no duplicate research areas
- c. first come first serve
- d. honoring symposia limited to fall
- e. encourage round table discussions

4) COMP advertising
- a. COMP Programming on twitter
- b. used for dissemination of programming information

5) PACS system will be migrated to OASIS system (not OASYS) 2014

6) Routine updating of the web page is taking place to include
- a. award winners and image contests
- b. programming information and guidelines

7) It should be reiterated that photos and recording of presentations and posters is not permitted.

8) Programming highlights for Philadelphia

Exploring Potential Energy Surfaces in Quantum Chemistry. A Tribute to H. Bernhard Schlegel

Hrant P. Hratchian (Gaussian, Inc) and Xiaosong Li (University of Washington)
The potential energy surface (PES) provides a central interconnect for the experimentally observed behavior of molecular systems and the theoretical description of that behavior. Indeed, the shape and contour of the PES dictate the structure and dynamics of molecular systems, and most spectroscopies can be studied as a response of the PES to one or more external perturbations. From geometry optimization to ab initio molecular dynamics, the development of

efficient PES exploration methods tailored for quantum chemistry have played a crucial role in expanding the applicability and importance of modern computational chemistry in scientific studies. This symposium honors H. Bernhard Schlegel on the occasion of the 30th anniversary of his landmark “Berny Optimization” paper [*J. Comp. Chem.*, **3**, pp214-218 (1982)], and will explore the current state of the field. Discussion topics will include new developments in geometry optimization, ground and excited state dynamics, QM/MM energy surface exploration, and novel applications of such techniques for investigating and understanding chemical questions.

Drug discovery in tyrosine kinase inhibitors and drug resistance

J. Phillip Bowen (Mercer University) & Haizhen Zhong (University of Nebraska – Omaha)
Significant progress has been made in the past three years in small molecule design that target pathways critical in angiogenesis. Aberrant angiogenesis – the formation of new blood vessels from pre-existing blood vessels and vascular endothelial cells – has been observed in many disease states, including inflammation, peptic ulcers, and cancer. In recent years, there are more than 10 tyrosine kinase inhibitors approved by the FDA as anticancer therapeutics, including gefitinib, erlotinib, dasatinib, sunitinib, sorafenib, lapatinib, pazopanib, and etc. There are more than 19 kinase inhibitors targeting EGFR and VEGFR entering clinical trials. VEGFR (vascular endothelial growth factor receptor) and EGFR (endothelial growth factor receptor) are two important enzymes regulating tumor growth and metastasis. Although these VEGFR/EGFR inhibitors are very effective against lung, breast, colorectal, and renal cancer, mutations do evolve. The evolving mutants reduce the sensitivity of cancer cells toward the above therapeutic agents.

This symposium will provide a platform for scientists to discuss approaches to circumvent or overcome mutations observed in VEGFR/EGFR kinase. This forum should provide effective communications in advances in this important research area and will assist scientists in the design of the next generation of efficacious tyrosine kinase inhibitors against resistant strains.

Recent Advances in Studies of Molecular Processes at Liquid Interfaces

Liem X. Dang (Pacific Northwest National Laboratory) & Hongfei Wang (Pacific Northwest National Laboratory)
Reactions that proceed at interfaces are also highly dependent on the interactions between the interfacial solvent and solute molecules. The interfacial structure and properties of molecules at interfaces are generally very different from those in the bulk liquid. Therefore, the chemical and physical properties of heterogeneous systems are dependent on understanding of the fundamental molecular interactions that give rise to interfacial molecular structure. This symposium brings together a group of scientists actively working on the development and/or improvement of techniques that describe the solvation in heterogeneous environments (*i.e.*, liquid/vapor and liquid/liquid interfaces). All of the advances offer new possibilities in addressing a wide range of problems in many disciplines, such as physical science, chemical physics and materials research. The purpose of this symposium is to feature both state-of-the-art theoretical and experimental techniques for understanding chemistry and solvation at liquid interfaces, and to explore new applications of these methods. Possible topics for the symposium include, but are not limited to, reactions at liquid surfaces, ion distribution, spectroscopy, vibration relaxation, and solvation effects. We expect a large attendance at this symposium from scientists and students from several disciplines and this symposium will facilitate fundamental research as well as advanced scientific education.

Recent advances in Quantum Monte Carlo

Emanuele "Manny" Curotto (Arcadia University)

Simulations of crowding, confinement, and cellular environments

Michael Feig (Michigan State University)
Computational studies of macromolecular systems are often carried out with single molecules at infinite dilution whereas realistic environments are more complex. In particular, biological environments present a significant degree of crowding and confinement due to very high

concentrations of nearby biomolecules. While this subject has been studied for some time, there is now renewed interest following new experimental data, increasing computer power, and advances in computational methodology. The goal of the symposium is to discuss recent computational studies in this area covering both biological and non-biological crowded and confined environments. It aims to provide a broad perspective in terms of both physical chemistry and computational methodology.

Scripting and Programming: Drug Discovery and High Performance Computing in the Cloud

Brian Moldover (B-Tech Consulting, Ltd) & Zheng Yang (Boehringer Ingelheim Pharmaceuticals Inc.)

Continuum Solvation Modeling in Biological Systems: Developments and Applications

Ray Luo (University of California, Irvine) & Emil Alexov (Clemson University)
Continuum solvation modeling offers a unique opportunity for more efficient biomolecular simulations without the loss of atomic-level resolution for biomolecules. New methods and new ideas in continuum solvation, coupled with developments in sampling algorithms, classical force fields, and quantum approximations, are proven to be useful for the entire biomedical community in a broad range of studies of biomolecular structures, dynamics, and functions. Our planned symposium “Continuum Solvation Modeling in Biological Systems: Developments and Applications” offers a platform for developers and other practitioners to exchange ideas to further our community wide efforts in this field. We anticipate that the symposium will cover various aspects of continuum solvation modeling in molecular biology including methodology developments, applications, and computational and theoretical approaches to model the roles of electrostatics in particular reactions in molecular biology.

Multiscale Modeling of Biomolecular Systems

Payel Das (IBM Thomas J. Watson Research Center) & Silvina Matysiak (University of Maryland)

CSAR 2011-2012 Benchmark Exercise

Heather A Carlson (University of Michigan) & James B Dunbar Jr (University of Michigan)
In late 2011, CSAR initiated a blinded exercise to provide members of the docking and scoring community an opportunity to test their methods. The unpublished data sets were provided by two pharmaceutical companies and colleagues at the University of Michigan, Ann Arbor. Participants provided both docked poses and affinity predictions. The exercise closed in the spring of 2012. Results for that exercise will be presented, and individual groups will discuss the insights gained through their participation.

Characterization and Screening of Databases of Porous Materials

Maciej Haranczyk (Lawrence Berkeley National Laboratory) & Michael W. Deem (Rice University)
Crystalline porous materials are an exciting group of materials with many current and even more envisioned applications. They can be used, for example, as catalysts or as materials for separations and storage of chemical species. This symposium will be focused on tools and approaches that are being developed in order to the search enormous chemical space of these materials and discover the best structures for these applications.

The list of to-be-discussed topics includes: (a) enumeration and prediction of crystal structures of porous materials; (b) methods and tools for computational characterization of materials; (c) novel structure representations and their applications to materials’ similarity, diversity selection and classification; (d) material databases and search engines; and (e) high-level approaches and case studies combining any or all of (a)-(d).

Understanding and Predicting the Role of Water in drug design

Jean-Francois Truchon (Chemical Computing Group, Inc), Vijay Panda (Stanford University) & Raul Alvarez (Chemical Computing Group, Inc)
Can we improve drug design with better computational treatment of water? Theories and methods will be explored, assessing evidence and validation techniques on the role of structured water in protein:ligand interactions.

Standing Invited Symposium

Perspectives in Applied Computational Methods

9) Anyone interested in organizing a symposium, please contact Emilo.

10) If we invoke a limitation in the number of talks per meeting, will we end up needing to be more selective on what is allowed to be presented?

a. we will see how things go and make decisions as needed

Fall ACS Meeting
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4:00-6:30PM

Attendees
Emilio Esposito, Ed Sherer, Jeffry Madura, Orlando Acevedo, Kennie Merz, Kate Holloway, Jane Tseng, Ralph Wheeler, Wendy Cornell, Terry Stouch, Chris Harwell, Rigoberto Hernandez, Luke Achenie, Petrina Kamya (CCG), Peter Jurs

Executive Meeting

4:00 – 4:05 Welcome – Jeffry D. Madura

4:05 – 4:15 Secretary Report – Ed Sherer

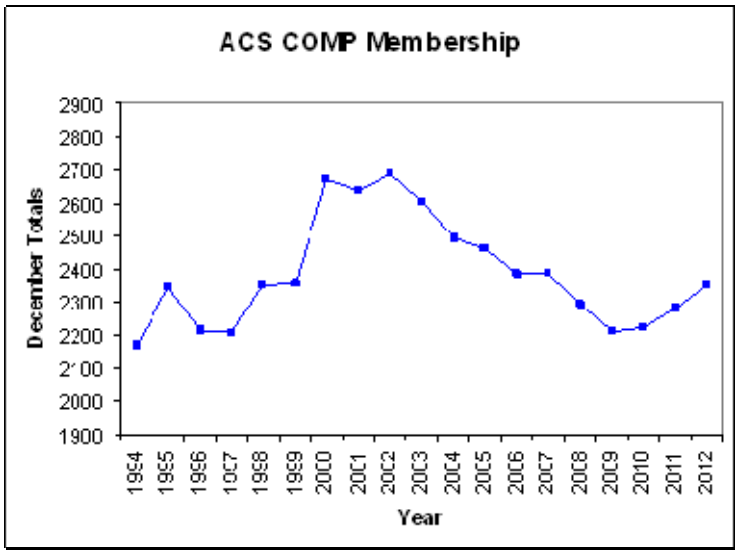
1) Election 2012: This year, COMP needed to fill the following positions: Chair-Elect to serve as Chair in the year 2014, and 2 Councilors: where the two people receiving fewer votes in the Councilor (2013-2015) vote will serve as Alternate Councilors (2013-2015). After the election, it was determined that Terry Stouch will be the new Chair-Elect for 2014. For the 2013-2015 period, Peter Jurs and Melissa Landon will serve as Councilors with Rommie Amaro and Rigoberto Hernandez serving as alternate councilors.

2) Vote on acceptance of meeting minutes: All outstanding minutes from past 3 years need to be approved after having been sent out after Spring 2012 meeting.

A motion was made to accept the minutes listed below (Chris Harwell)
The motion was seconded by Jeffry Madura and the vote to accept was unanimous.

Minutes accepted:
Spring 2009
Fall 2009
Spring 2010
Spring 2011
Fall 2011
Spring 2012

3) Membership Update 2012: membership is continuing to increase up 71 members from 2011.



4) Finally, Steven Trohalaki sent a thank you letter to COMP for helping to fund the 43rd Regional Meeting of the ACS in Dearborn, MI.

4:15 – 4:30 Treasurer Report – Chris Harwell / Sara Nichols

1) The financials are in good order

2) The shipping of ARCC was substantially larger this year than last, Chris and Ralph to look into this.

3) $500 will be donated to help run the CCL

4) Councilors should get their expenses to Chris as soon as possible

5) The American Funds CD has been closed and monies moved to COMP's account.

6) Funding of the Pharmaceutical ACS award is going to be an issue. COMP either needs to find another sponsor, or consider funding this ourselves. Kennie is looking into some options. PHYS is also having a hard time funding their awards and may need to fund themselves. Endowing the award would cost $450K. Contact at ACS is Felicia Dixon.

7) Dues are usually set at the same level. Currently $16/full and $7.50/students. Our allocation this year was much lower, we could consider filling some of this in with dues. One possibility would be comparing to other divisions dues levels. Owing to our increasing membership and the state of the economy, possibly leave the dues at the current level. MEDI dues are $25. It could be possible to raise dues slowly each year,

maybe $1 so that you can avoid a larger shift down the road. Dues have not risen since at least 2009. The dues level may have been dropped before that.

A note to consider is that ARCC will not lower cost of publication for purely electronic since there is a hosting cost.

In the 2012 ARCC survey it was determined that 20% of the membership wanted paper copies, 42% wanted electronic, and 32% wanted both.

ACTION ITEM: Discuss dues at retreat and vote on changes during Spring meeting.

4:30 – 5:00 Programming Report – Emilio Esposito / Scott Wildman

1) San Diego meeting had 45 withdrawals. COMP paid for 63 registrations based on organizers and presiders.

2) Philly has 567 abstracts, with 40 withdrawals.

3) COMPs allocation is dependent on the number of members who get scanned at the Expo, also on the maximum number of attendees at the symposia.

3) Abstract acceptance policy

4) Limitation to number of presentations per person

5) COMP has a new sponsor for the drug discovery sessions: Cresset.

5:00 – 5:15 TDT – Wendy Cornell / Jane Tseng Hanneke Jensen

1) Discuss the TDT

Initiative is funding travel, registration and purchasing of compounds from eMolecules for award winners. Compound purchases will be for benchmarking the computational work which was submitted.

2) TDT is making a request to COMP for funding. Wondering whether COMP would like to consider matching funds to the Innovative Grant which TDT received from ACS. A match of 50% would be around $3700. A second social event would take about $1000, the remainder would be for compound acquisition. Networking event would be in New Orleans.

Currently there are about 100 subscribers to the TDT newsletter and about 60 have downloaded the data sets.

5:15 – 5:30 CCG Awards – Petrina Kamya

1) Petrina organizes the CCG Excellence Awards.
    a. CCG would like to know the number of applicants for these awards
    b. Carlos is the organizer and would have these numbers, recommendation is to contact Carlos
    c. $500 additional travel award added to the overall award

5:30 – 5:45 Councilor's Report – Peter, Ralph, and Emilio

1) Peter – Elected Committee of Council, council policy committee and sets agendas for committee meetings. Peter is able to put items on to the council meeting agenda on behalf of COMP. Most work done in separate committees and then that work is then approved by council.

Three important committees are:

Nominations and Elections
Committee on Committees – staffs all ACS committees
Council Policy Committee

2) Ralph – Committee on Science. Organizing symposia outside of the purview of normal divisions. Alternate energies, solar, biodiesel, entrepreneurs forum. Ralph is a candidate to be on the committee on committees.

3) Emilio – Meetings and Expositions. A new policy for losing your badge is to get one free, and then losing after is $25, $50, then $100 everytime after.

Registration for next year 2013 will be $380. A $20 increase over 2012.

Currently the proposal is for a registration increase to take place to cover the cost of recording all content to be deposited on the web. But you could opt out of the talks possibly.

Vendors can sign up for a virtual booth if they want to just do electronically.

ACS considering satellite exhibitions which would be spread out tables/booths within the meeting space.

COMP recommendation to the MME is to have more regular and extended transportation for large spread out convention venues.

4) Luke – MPPG, theme for San Francisco 2016 is computers in chemistry, sharing data, databases, verification, and validation. What are future software needs? How does social networking play into chemistry. Quantum computers.

Should COMP nominate a person to help design the strategy for getting COMP relevant topics into this overall theme?

5:45 – 6:00 ARCC – Ralph Wheeler

1) Coming volume will be ready for publication in October, will be 6 chapters on method development.

ACTION ITEM: Jeffry will look into alternatives for electronic publishing by the retreat 2013.

6:00 – 6:30 Old Business – Jeffry D. Madura

A) unknown whether mentor lunches will take place in Philadelphia

1) Undergraduate update (list too long, able to give ribbons/certificate)
    a. Jeff Evanseck is contact for undergraduate development
    b. 3 COMP chem. posters in the undergraduate symposium
    c. Kate, Ed, and Jeffry will participate in the undergraduate mentoring sessions Monday morning
    d. Is COMP willing to fund a travel award for undergraduate posters
        1. some divisions give up to 10 travel awards
    e. another option would be to fund travel prospectively by taking applications in advance
    f. Certificate, copy of ARCC, membership for one year, ribbon for badge
        1. give up to 10% of the number of posters

2) Co-sponsorship with ChemEd.

3) Brown bag lunch in New Orleans to connect with undergraduates

Jeffry and Jeff will define something and bring back to COMP.

4) CCG-like awards for undergraduates? (Universities to take the lead?)

Peter makes a motion that COMP awards up to 10% of the undergraduate posters submitted (and tagged as COMP) to include ribbon, ARCC, COMP membership for 1 year, cash of $100, and award will be called: "COMP Undergraduate Poster Award" where name can be amended in future with sponsors, etc.

Kate seconded the motion.

The vote was passed unanimously.

5) ACS Graduate & Postdoctoral Scholars Reception

Monday night. We paid to be part of this. Jeffry and Ed will attend.

6) ACS Award for Computers in Chemical and Pharmaceutical Research

It was pointed out again that this award seldom goes to Pharmaceutical employees.

Mentioned earlier in the meeting, Kennie will be pursuing angles on getting this award endowed.

7) Matching of innovative grants
   a. will COMP agree to match a certain value moving forward?
   b. up to 50% by reasonable request
   c. not automatic, COMP will still need to weigh each option
   d. request should be made ahead of time, prior to grant submission

Vote:

Kennie makes the motion that we fund TDT at $3700, which was seconded by Ralph.

The vote was passed unanimously.

8) Carlos is no longer going to be a councilor, but will continue as the award coordinator.