

Present: John Straub, Ken Jordan, Bruce Kay, Jim Skinner, Anne Chaka, Krishnan Raghavachari, Jan Steckel, and Don Truhlar

Items Discussed:

1. Status of subdivision officers: Select Committee to choose next Vice Chair (service to begin 8/05). Ken Jordan and Anne Chaka agreed to serve on the committee. Dave Freeman was suggested as a third member of the committee. John Straub will contact Dave to find out if he will serve. Names of candidates for Vice Chair (for committee to consider) were suggested including Angela Wilson and Anne McCoy.

2. The newsletter was discussed; next newsletter should be issued within a month or so and will contain the names of the IBM graduate student awards. As a way to help garner support for the IBM awards, for which funding seems in danger once again, it was suggested that it might be worthwhile to compile a history of the graduate student awards that would include the students who have won it in the past and maybe a little information about what those people are doing now. Jan Steckel will attempt to compile this information.

Jan Steckel asked those present whether it is worthwhile to attempt to continue the symposia summaries, as it is difficult to get contributions for this. The general discussion seems to favor attempting to continue this.

The newsletter was sent electronically only and it seems this method of distribution is favored. Other items for inclusion in the newsletter will be calls for papers for Atlanta and San Francisco. It was noted that submission of papers for Washington will close soon after the San Diego meeting ends.

3. Status of the website: Our webmaster, John Adams, could not attend the subdivision meeting due to other ACS duties but the website was discussed. Jan Steckel has been in contact with John regarding updates or corrections to information on the website and he readily makes corrections that are sent to him. When a list of all the past IBM graduate student awardees has been compiled by Jan Steckel, it should be added to the website.

4. The status of the IBM graduate student awards was discussed. Krishnan will meet later this week with Sharon and this year's awardees will be chosen. Krishnan will send information to Jan Steckel for inclusion in the newsletter. A more worrisome topic was the fact that funding for IBM for next year is uncertain. Several ideas for alternative funding sources (Intel, Phillip Morris, Altra) were mentioned.

5. Funding for the Langmuir Award, which has been provided by GE, is uncertain.

6. JPC A and JPC B are not the same 'size' and perhaps there is a perception that JPC A is not as "successful" as JPC B; there are proposals to move certain topics (biophysical, liquid state) from JPC B to JPC A.

7. Ideas for new symposia were discussed.

A DFT symposia in honor of Bob Parr has been suggested by Weito Yang; it would have to be co-sponsored by COMP in order to be "in honor of".

Jiansho Cao has proposed a symposium titled "Advances in condensed phase quantum dynamics: Theory and new applications"; quite a few names were suggested as possible coorganizers.

New ideas for symposia include: electronic structure of complex materials (zeolites, etc), accelerated dynamics, nanostructured materials, computational electrochemistry (possible organizer: Bruce Garret), multiscale modeling/whole cell modeling/systems biology.

Computational photochemistry was suggested as an idea for a future symposium; this could include topics such as solvent effects on photochemistry, excited states, dynamics, and Todd Martinez was suggested as a potential organizer.