

**The Molecular Graphics and Modelling Society**  
**34rd Annual General Meeting**

*15<sup>th</sup> April 2015, 5.20-6.00pm, Simpkins Lee Lecture Theatre, Lady Margaret Hall, The University of Oxford, Membrane Signalling and Transport: Computation and Experiment*

**CHAIR'S REPORT**

The Molecular Graphics and Modelling Society is a charitable society that was formed in 1981 with the aim of promoting education and research into molecular graphics and modelling. One of the main ways of achieving this principle aim is through the organization of scientific meetings and workshops such as this current "Membrane Signalling and Transport: Computation and Experiment" meeting held here in Oxford. I would like to extend my thanks to the members of my research group and LMH who have helped in the organization of this particular meeting.

The timing of the AGM is dependent on which meetings are being organized and hence this years AGM is relatively soon after the last AGM which was held in August 2014. Nevertheless I am happy to report that the Society has continued to be active during that short time, despite the tough financial conditions. The main event since August last year has been the annual Young Modellers Forum, which as usual provided an excellent showcase of talented modellers and highlights the real strength the UK and indeed Europe has in this scientific field. The exposure to industrial colleagues that this event provides to young scientists is still unique in the conference world and I am very proud that the MGMS continues to organize this event and does so to such a high standard. It is particularly important at a time when participation at conferences and events by industrial colleagues is somewhat limited by financial restrictions in the present climate. There was strong competition for the coveted 12 poster and 12 oral presentation places. The names of the winners for the best oral and poster presentations can be found on the MGMS website. My particular thanks are extended to Steve Maginn not just for his organization of this year's event, but also for all of his hard work over the many years that he has taken on this responsibility. It is thanks to Steve that the present shape and form of the meeting is so streamlined and successful. Steve will act as a shadow on the 2015 YMF to help ensure a smooth transition, but there is no doubt that he will be sorely missed at the YMF. Thankfully, he will continue in his role as membership secretary.

As the past year has been another active one for the MGMS, there is much to look forward to in the year ahead including the YMF on the 27 November in London. This year we are experimenting with moving the event to the University of Greenwich and I would like to thank Jiayun Pang for her efforts in making this happen. The MGMS is also happy to be organizing a meeting in Singapore this year, also in November (25<sup>th</sup> to 27<sup>th</sup>). My thanks go out to Peter Bond and Chandra Verma for hosting this at Biopolis and putting together an extremely impressive list of speakers. We will also be organizing jointly with the Chemical Structure Association, the 7<sup>th</sup> Joint Sheffield Conference on Chemoinformatics on the 4-6<sup>th</sup> July 2016. I would like to extend my thanks to Val Gillet for organizing this yet again. It is always a very popular and successful event and I have no doubt this trend will continue next year.

Another activity the Society organizes is a Lecture Tour by a prominent computational chemist or modeller. Last year saw an excellent tour from Professor Art Olson, which was extremely well received. This year it is my pleasure to announce that Professor Gisbert

Schneider of the ETH Zürich will be delivering the lectures. The exact timing and dates will be announced shortly.

The sponsorship of prizes is another important way in which the Society seeks to promote computational chemistry. The prestigious MGMS Silver Jubilee Prize is awarded each year to outstanding young researchers in the field. We have not started the process for this year's prize, but that will begin shortly after this meeting comes to an end and I am very confident we will see a very highly competitive field again.

The success of these activities, which play a vital role in promoting computational chemistry and the cohesiveness of its community, are underpinned by the generous sponsorship of companies and organisations but also the tireless involvement of local meeting organisers and MGMS committee members. The work of the Society depends on the hard work of these volunteers. At this meeting, Frank Blaney and Jonathan Hirst have chosen stand down as members of the committee. I would like to thank them both for their contributions to the MGMS over the past years. Both of them have contributed an incredible amount over the years and their involvement will be sorely missed. I would also like to thank Christine Richardson, a previous chair and co-opted committee member, who will also be leaving the committee.

The previous AGM saw quite a change in committee members and would like to thank all of them for their commitment, enthusiasm and support over past year. My particular thanks go to Garrett Morris and Brendan Howlin for their hard work as Secretary and Treasurer respectively. As I am sure Brendan will elaborate, the transfer of the Treasurer position has been hindered considerably by what can only be described as incompetence by HSBC, the society's bank. That has led to a considerable delay in preparing the accounts this year. However, we believe we have resolved all of the issues and so things should return to normal in the next few days if they have not done so already.

As the Society enters its 35<sup>th</sup> year, I can confidently report to this Meeting that the MGMS continues to make a significant impact in developing and promoting computational chemistry, through its meetings, lecture tours, prize and other activities. The Society exists for the computational chemistry community and depends on your support. There are many ways to become more connected to the MGMS, by visiting our website ([www.mgms.org](http://www.mgms.org)), joining our LinkedIn group ("Molecular Graphics and Modelling Society") and primarily through becoming a member. If you would like to find out more about the Society or make suggestions around meetings that you would like to see and get involved with, then please do contact myself or other committee members.

Philip Biggin

April 2015