

The Molecular Graphics and Modelling Society

35th Annual General Meeting

Monday 4th April 2016, 5.30-6.00pm, The Edge Conference Centre, The University of Sheffield, The Seventh Joint Sheffield Conference on Cheminformatics.

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. The main vehicle for achieving this aim is through the delivery and support of scientific meetings and workshops such as this current "Seventh Joint Sheffield Conference on Cheminformatics" meeting held here in Sheffield. The fact that this particular conference is in its seventh iteration is a testament to the local team here who always manage to make this conference run with the smooth efficiency of a well oiled-machine and I would just like to first thank Val Gillett, John Holliday and Peter Willett for all their hard work and for kindly hosting this AGM as well.

I am very pleased to say that the MGMS has had another very successful year with two international meetings amongst its activities. The first of these was "Membrane Signalling and Transport: Computation and Experiment" held at Lady Margaret Hall in Oxford in April and was a vibrant and well-attended meeting with about 90 people. As the name of the meeting suggests, it brought together experimental and theoretical colleagues and spawned some nice new collaborations. I would like to thank publically members of my own research group and the team at LMH for their help in making that conference run so smoothly.

The second international meeting continued the theme of linking theorists with experimental colleagues and was called "Exploring Mechanisms in Biology: Theory and Experiment" and was held in Singapore at the end of November 2015. That conference was also a great success and I would like to extend my thanks to the organizers there, in particular Chandra Verma and Pete Bond.

Almost running simultaneously was the annual Young Modellers Forum held for the first time this year at the University of Greenwich on the 27th November. As usual, this provided an excellent showcase of talent 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 quite 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. I feel also that this kind of event is very important in the current financial climate when participation at conferences and events not only by students but also by industrial colleagues can be rather limited.

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 this year to Jiayun Pang who was ably supported by Louise Birch and Steve Maginn.

As we move forward, there are many exciting conferences planned, and the first of these is the "Big Data in Biomolecular Systems" which is a one-day meeting that will be held on 9th September 2016 at the London School of Pharmacy. My thanks go to Ewa Chudyk and Mike Mazanetz for putting this exciting program together and also to Evotec for co-sponsoring the event.

As well as the organizing and sponsorship of meetings and workshops, the MGMS also regularly holds lecture tours. 2015 saw a fantastic series of lectures delivered by Professor Gisbert Schneider, (ETH Zurich) at three locations: Imperial, Bristol and UCB. These lectures were very well attended and hailed a great success and I extend my thanks to the local organizers for hosting Gisbert during his tour. The next lecture tour speaker is not yet decided and so I urge MGMS members that if they have suggestions, the committee would be very happy to consider them at the next committee meeting.

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. This year as we just saw and heard, Peter Kolb was the deserving recipient. I once again offer my congratulations to Peter. And also to remind you that if you know anyone who is eligible, then please do encourage them to apply for next years award.

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. I would like to thank all of them for their commitment, enthusiasm and support over the past year. My particular thanks go to Garrett Morris and Brendan Howlin for their hard work as Secretary and Treasurer respectively. This year also saw the transfer of Editorship of the Journal of Molecular Graphics and Modelling from Jonathan Hirst to Jamie Platts. I thank Jonathan for his hard work over the years in making the journal a success and also judging the graphics prize which the journal runs every year. I am also grateful to Jamie for taking on the editorship and I am very confident that it is in good hands.

As the Society enters its 36th 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), 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.