

The Molecular Graphics and Modelling Society

38th Annual General Meeting

Monday, 17th June 2019, 5.30-6.00 pm, The Edge Conference Centre, Sheffield
UK.

CHAIR'S REPORT

Since its founding in 1981, the Molecular Graphics and Modelling Society has tirelessly promoted the education and research into the use and development of molecular modelling and computer graphics techniques. One of the main vehicles for achieving those goals has been through the support and delivery of scientific workshops and meetings such as this meeting "*The Eighth Joint Sheffield Conference on Chemoinformatics*". As the title says, this is the eighth in this particular series of meetings, which first started in 1998. Over those years the reputation of this meeting has become quite formidable, due to the fantastic organizational teams behind the scenes. This year is no exception and I would like to extend my thanks to Val Gillett, Peter Willett, Dave Winkler, Nathan Brown and Garrett Morris for what will no doubt be the best one yet!

I am pleased to report that the MGMS has had another very successful programme of events. The first to report on was the "*Discrete Models in Systems Biology*" meeting held on the 29-31st August in Murray Edwards College, Cambridge. This was a relatively new area for the MGMS in terms of the underlying subject material and the meeting created some new interactions between groups of people that were traditionally from different "camps". I would like to extend my thanks to Ben Hall, David Shorthouse and the rest of the team there for putting together a very interesting and rewarding program. I am sure this is an area that the MGMS will venture into more and more in the future.

Next and last in the calendar for 2018, was the "*Young Modeller's Forum 2018*" held for the fourth time at the University of Greenwich on the 30th November, 2018. The quality of presentations from students continues to be magnificent and is a testament to the young talent that is coming through in this field not only from the UK but also from the rest of Europe. The event is extremely well attended and supported by the industrial sector and I would just like to acknowledge and thank all those who generously supported it again this year. The support allows us to keep this event free to attend and even to provide some limited travel expenses.

As usual and in keeping with the reputation of this event, there was once again strong competition for the 12 poster and 12 oral presentation places. The winners of the talk prizes were Jonathan Shearer (University of Southampton), Francesca Vianello (Imperial College) and Timothy Burd (University of Oxford). The winners of the poster prizes were Joshua Carter (University of Oxford) and Silvia Amabilino (University of Bristol/NovaData Solutions). Congratulations to them all. My particular thanks are extended this year to Jiayun Pang and Mike Mazanetz, who were once again ably supported by Louise Birch and Steve Maginn. The 2019 YMF will be the next conference after this AGM and

will once again be held at the University of Greenwich on the 30th November 2019. We can look forward to another excellent day of science.

Earlier this year we held a one day meeting "*Big Ideas for Big Data in Drug Discovery*" at the UCL School of Pharmacy on the 12th April 2019. This meeting attracted a diverse set of attendees and there was plenty of discussion about how to deal with some of the problems around big data in general. I would like to extend my thanks to Shozeb Haider for being the local host and especial thanks to Ewa Chudyk who put together a fantastic day. I also extend a big thank you to our industrial sponsors for

that meeting. It is very much appreciated.

The sponsorship of prizes is another important way in which the Society seeks to promote computational chemistry and this year is no exception. In fact, this is a rather special year in terms of prizes as we were able to award the first “*MGMS Frank Blaney Award*”, which was previously known as the *MGMS Silver Jubilee Prize*, to Dr Christopher Rowley, who is based in the Chemistry Department at Memorial University of Newfoundland, St John’s, Canada. His group uses computer simulations to study biophysical chemistry and other complex chemical processes. Well done Chris! If you know someone who might be eligible for the prize next time, then please do encourage them to apply. Note that it is also possible to self-nominate, but you must find someone to write a letter of support. The process will begin in Autumn and as usual, full details will appear on the website in due course.

This year, the *MGMS Lecture Tour* was given by Dr David Glowaki (also the winner of the *MGMS Silver Jubilee Prize* in 2017). David gave, what is probably the most interactive lecture tour to date, as he was able to demonstrate the use of virtual reality in molecular modelling. My thanks to the various institutions around the UK that hosted David as part of that tour. The next lecture tour will be given by Professor Rebecca Wade, of the Heidelberg Institute for Theoretical Studies, later this year. If you would like to host Professor Wade, please get in touch with a committee member.

I would also like to draw your attention to a new initiative that the *MGMS* launched last month called the *MGMS Early Career Workshop Initiative*. This is a new mechanism to help encourage younger PIs and Post-docs to think of interesting and innovative ideas that might serve the community and to use the *MGMS* for support and advice to help make it work. It might be a meeting or a workshop or something completely novel. The deadline for the first call was the end of May, and at the time of writing this report, we were yet to announce the winners, but I am pleased to say we had an excellent set of submissions and perhaps I will be able to make an announcement at the AGM.

The work and success of the *MGMS* depends on the hard work of 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. My thanks also to Jamie Platts for all his hard work as Editor of the *Journal of Molecular Graphics and Modelling*. It would be great to see more members publish their work in this journal. I also thank Steve Maginn for his hard work as Membership secretary and for ensuring people are aware of conferences and workshops. I also thank Shozeb Haider for taking on the role of webmaster.

As the Society enters its 39th 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 for meetings that you would like to see and get involved with, then please do contact myself or other committee members.

Philip Biggin, Chair of the *MGMS*
June 2019