

The Molecular Graphics and Modelling Society

37th Annual General Meeting

Wednesday, 29th August 2018, 5.30-6.00 pm, Murray Edwards College,
Cambridge, UK.

CHAIR'S REPORT

The Molecular Graphics and Modelling Society was founded in 1981 as a charitable organization with the key goal of promoting education and research into scientific endeavours that develop or utilize molecular modelling and computer graphics techniques. Historically and still very much to this day, the main mechanism for achieving that goal is through the delivering and support of scientific meetings and workshops such as this current "*Discrete Models and Formal Verification in Biology*" meeting held here in Murray Edwards College, Cambridge. At this point in time, I'd like to extend my thanks to Dr Ben Hall for his organization of this meeting, which looks like it will be a great success.

This past year has been another very successful one for the MGMS with several well-attended meetings. The first was a one-day meeting held at the School of Oriental and African Studies (SOAS) titled "*MD in Pharma*" on the 11th April 2017 and brought together many leading exponents of molecular dynamics in both the pharmaceutical industry and academia. I would like to extend my thanks in particular to Ben Cossins and the three sponsors (UCB, Boehringer Ingelheim, and Schrödinger) for making that meeting so successful.

The second meeting was a three-day meeting focused on "*QM/MM Methods and Applications*" held on the 4-6th September, 2017, at the University of Manchester. This was another very successful and timely meeting and highlighted the strength and depth of this subject within the UK and Europe in general. My thanks to Richard Bryce, Sam De Visser and Sam Hay for putting together an excellent program and a smooth-running event.

The final event of 2017 was the "*Young Modellers' Forum 2017*" held for the third time at the University of Greenwich on the 24th November, 2017. The standard of presentations at this event continues to be excellent and serves as a fantastic showcase of the young talent that is coming through in this field not only from the UK but also from the rest of Europe. It continues to be well attended and supported by the industrial sector and provides an excellent opportunity for rich interactions to develop between industrial and academic researchers.

There was strong competition for the coveted 12 poster and 12 oral presentation places. The winners of the talk prizes were Adam Baskerville (University of Sussex), Hannah Bruce Macdonald (University of Southampton) and Nick Fowler (University of Manchester). The winners of the poster prizes were Marc Daemgen (University of Oxford) and Ricardo Parra-Cruz (University of Nottingham). My particular thanks are extended this year to Jiayun Pang, who was once again ably supported by Louise Birch, Steve Maginn and Mike Mazanetz.

The 2018 YMF will be the next conference after this AGM and will once again be held at the University of Greenwich on the 30th November 2018. My thanks in advance once again go to Jiayun Pang and this year also to Mike Mazanetz, Louise Birch and Steve Maginn.

On the 11th and 12th of April 2018, the MGMS partnered with the UK-QSAR and cheminformatics group to host a joint meeting entitled "Structure-Activity Relationships" at the University of Cardiff. This was a very well attended meeting and thoroughly enjoyed by all concerned. My thanks to Steve Maginn, Jamie Platts and Brendan Howlin and colleagues at UK-QSAR for such a splendid and smooth-running conference.

Shortly after this meeting we were all deeply saddened to learn of the passing of Dr Frank Blaney on the 14th April 2018. Frank was a founding member of the MGMS and remained intimately connected to it ever since. He served as Chair of the MGMS and was also responsible for the organisation of many successful conferences throughout his life. He was a long-standing member of the computational chemistry community and had a particularly strong interest in membrane proteins including GPCRs, ion channels and transporters. He also had an interest in using QM methods to understand cytochrome P450s. Following a long career at GSK, his interest and substantial expertise in GPCRs led to his becoming a consultant, working closely with Heptares Therapeutics. He was a font of knowledge for computational chemistry and we will all miss him very much indeed.

The sponsorship of prizes is another important way in which the Society seeks to promote computational chemistry. The prestigious *MGMS Silver Jubilee Prize* (in its 10th year) was awarded to Dr David Glowacki for his excellent work on interactive visualization. My congratulations to him. Given the interactive nature of his work (using virtual reality headsets etc), the MGMS is pleased that Dr Glowacki will give a mini lecture tour so please go along if you get the opportunity to see and interact with molecules!

In recognition of Frank Blaney's work with the MGMS, the committee was unanimous in their approval that the *Silver Jubilee Prize* be renamed "*The Frank Blaney Prize*". 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. We will begin the process this autumn. Full details will appear on the website shortly.

The MGMS also regularly holds lecture tours. Dr Andrew Leach of the EMBL EBI has commenced his lecture tour and has already visited Manchester. The lectures at Southampton and Dundee are still to take place so keep your eyes out for those events.

The success of these activities, which play a vital role in promoting computational chemistry and the cohesiveness of our 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. 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 Stuart Firth-Clarke for all his efforts in keeping the website up to date and for Shozeb Haider for offering to take this on this year.

As the Society enters its 38th 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

July 2018