The Molecular Graphics and Modelling Society
36th Annual General Meeting
Monday 4th September 2017, 5.30-6.00pm, Manchester Institute of Biotechnology,
University of Manchester, 131 Princess Street, Manchester, M1 7DN.

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 "QMM Methods and Applications" meeting held here in Manchester. This is not the first time that Manchester has hosted an MGMS meeting on Quantum Mechanics and I am quite sure it won't be the last. I am also sure this current meeting will be a roaring success and for that I would like to extend my thanks to the organizing team here, but in particular Richard Bryce, Sam De Visser and Sam Hay.

I am very pleased to say that the MGMS has had another very successful year in 2016 with two international meetings amongst its activities. The first of these was the "Seventh Joint Sheffield Conference on Chemoinformatics" held at the University of Sheffield, UK, 4th-6th July 2016. This was another excellent meeting and the fact that it is in its seventh iteration is a testament to the world-class reputation of Sheffield and the excellent organizational skill of the team there. I extend my thanks to all involved in that meeting but in particular Val Gillet, John Holliday and Peter Willett.

The second meeting was a one-day meeting entitled "Big Data in Biomolecular Systems" held on the 9th September, 2016, at the School of Pharmacy, UCL, London. This was another very successful and timely meeting that highlighted the many different aspects of "Big Data" that are starting to feature in areas such as functional genomics, network pharmacology, biosimulation and chemical data collections. My thanks to Ewa Chudyk and Mike Mazanetz for putting together an excellent program and a smooth-running event. I also thank Shozeb Haider for hosting us at the UCL School of Pharmacy.

The final event of the year was the Young Modellers Forum held for the second time at the University of Greenwich on the 25th November, 2016. The standard of presentations at this event continues to be extremely high 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. As I mentioned last year, I feel this kind of event is very important in the current financial climate when participation at conferences and events not only by students but also be industrial colleagues can be rather limited.

There was strong competition for the coveted 12 poster and 12 oral presentation places. The winners of the talk prizes were Richard Lewis (Cambridge), Joshua Meyers (ICR) and Vladimiras Oleinikovas (UCL). The winners of the poster prizes were Julian Gaberle (UCL) and Fiona Naughton (Oxford). My particular thanks are extended this year to Jiayun Pang, who was once again ably supported by Louise Birch and Steve Maginn, and for hosting us at the University of Greenwich.

The 2017 YMF will be the next conference after this AGM and will once again be held at the University of Greenwich on the 24th November 2017. My thanks in advance go to Jiayan Pang and this year also to Mike Mazanetz, Louise Birch and Steve Maginn. This will be followed by a joint MGMS/UK-QSAR meeting at the University of Cardiff on 11-12th April, 2018.

As well as the organizing and sponsorship of meetings and workshops, the MGMS also regularly holds lecture tours. There was no tour in 2016, but this year we are very honoured and pleased that Dr Andrew Leach of the EMBL EBI has agreed to give the next tour, which will be in Autumn 2017, and will feature Southampton, Bristol, Manchester and Dundee. This should be a very interesting series of lectures and I hope as many of you can attend one of these. Keep an eye on the MGMS website and the mailing list for details of the dates.

The sponsorship of prizes is another important way in which the Society seeks to promote computational chemistry. The prestigious MGMS Silver Jubilee Prize was slightly delayed this year and thus will feature in the 2017 report rather than this one, but may I take this opportunity to remind you that if you know anyone who is eligible, then please do encourage them to apply for next year's award – we will begin the process this autumn. Note that it is also possible to self-nominate, but you must find someone to write a letter of support. Next year will be our10th Silver Jubilee Prize. The closing date for nominations is 27th October, 2017.

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.

As the Society enters its 37th 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 2017