



The Molecular Graphics and Modelling Society

36th Annual General Meeting

Monday, 4th September, 2017, at 5 pm

Manchester Institute of Biotechnology Lecture Theatre, The University of Manchester, 131 Princess Street, Manchester, M1 7DN, UK.

<http://www.mib.ac.uk/contact/>

AGENDA

1. Minutes of the 35th AGM held at the The Edge, Endcliffe Village, 34 Endcliffe Crescent, Sheffield, S10 3ED, UK.
 - The minutes were approved.
2. Matters arising
 - There were no matters arising.
3. Chair's Annual Report
 - PB presented the 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 by 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 our 10th 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.”

4. Secretary's Annual Report

GMM presented the MGMS Secretary's Report:

“In addition to the current meeting, the MGMS has been involved in the organisation and support of the following events over the last year:

- o 7th Joint Sheffield Conference on Chemoinformatics, University of Sheffield, UK. 4th – 6th July, 2016.
- o Big Data in Biomolecular Systems, School of Pharmacy, UCL, London. 9th September, 2016.
- o Young Modellers' Forum 2016, University of Greenwich, London, UK. 25th November, 2016.

We would like to thank everyone who helped run these events, the sponsors, and all of you who attended.

Please keep an eye on our website and LinkedIn page for details and get in touch if you would like any further information.

Composition of the MGMS Executive Committee: The composition of the current committee/trustees is given below (dates of election are given in parentheses).

Chairman	Phil Biggin (2016)
Secretary	Garrett M. Morris (2014)
Treasurer	Brendan Howlin (2015)
Membership Secretary	Steve Maginn (2016)
Meetings Secretary	—
Journal Editor	Jamie Platts (2016)
Ordinary Members (7)	Richard Bryce (2014)
	Stuart Firth-Clark (2014)
	Shozeb Haider (2014)
	Val Gillett (2015)
	Jiayun Pang (2015)

	Irina Tikhonova (2015)
	Adrian Mulholland (2016)

Many thanks to all of the committee for their hard work over the year.

Co-opted members for the current year were: Louise Birch, Ewa Chudyk, Tim Clark, Ben Cossins, Xiao Lewell, Mike Mazanetz, and Dave Winkler.”

5. Treasurer’s Annual Report

Brendan Howlin, MGMS Treasurer has a submitted detailed report which is available by contacting the Secretary, and presented this report, including the following highlights:

(1) Proportion of profits from MGMS Sponsored meeting: MGMS meeting "Exploring Mechanisms in Biology: Theory and Experiment" held in Matrix (A*STAR) Singapore from 25-27 November 2015. SGD 8250/- or £4670; (2) MD in Pharma, sponsored by UCB, Portion of Profits, £5400; (3) Currently in the process of transferring our bank accounts to CAF Bank owing to dissatisfaction with HSBC; (4) Current balances as of 10/07/17: Current : £40,581.81, & Savings: £17,237.10.

6. MGMS Membership and Fees

Steve Maginn, MGMS Membership Secretary, presented the following report:

“MGMS membership currently stands at a high figure of 219. All members who joined in 2015 and have not renewed have been removed from the list, and those who joined through attendance at the MD in Pharma meeting in April 2017 have been added (60 people). Members who joined through the Sheffield Chemoinformatics meeting (83 people) and the Big Data meeting (28 people) in 2016 will remain on the list until the end of this year, and if they do not renew for 2018, will be removed at that point. Conference / meeting attendance remains the biggest source of members for the Society. We have now removed the option of paying for a physical copy of the Journal of Molecular Graphics and Modelling through membership.

Regular emailings of items of interest to the membership (relevant job opportunities, relevant non-commercial conference notifications, society news etc.) are now being sent through a webmail address, membership@mgms.org . This address may also now be used for correspondence with the Membership Secretary rather than a personal email address, providing continuity for when the holder of the post changes. Many thanks to Stuart Firth-Clark for setting this up.”

7. The Journal of Molecular Graphics and Modelling Society

The following report was submitted by the Editor of the JMGM, Jamie Platts:

“We are saddened to report the sudden and unexpected death of Dr Jeffrey Madura in March 2017. Jeff had been editor of JMGM since 2009, and was hugely influential in shaping its success. Elsevier plan to reinstate the “Best Graphics” prize and name this in honour of Jeff’s memory. Announcement of the prize will be made early in 2018. Negotiations for a successor, nominated by ACS Comp Division, are ongoing. For now, Dr Platts is sole editor.

Submission numbers continue to grow, and are on course for around 800 for 2017 (cf 600 in 2014). Acceptance rates are stable at around 25-30%, and production times are down slightly due to technical improvements with Elsevier. Impact Factor is down slightly to 1.75, continuing a steady downward trend from above 2 a few years ago. Submissions from MGMS members would be very welcome!

Submissions welcome from all aspects of molecular modelling and computational chemistry. Full paper or short communication. Also review articles or commentaries. Fast publication: 3.7 weeks submission to first decision; 7 weeks submission to final decision; 2 weeks acceptance to citable online; and Open Access is available.”

8. Election of Trustees/Committee Members and Chair

- Retiring: No-one.
- Re-standing: Garrett M. Morris (Secretary), Stuart Firth-Clark (Ordinary Member), Richard Bryce (Ordinary Member), and Shozeb Haider (Ordinary Member).

The elections took place, and Garrett M. Morris was re-elected as Secretary, Stuart Firth-Clark, Richard Bryce, and Shozeb Haider were re-elected as Ordinary Members.

Following the AGM elections, the Committee consists of:

Chairman	Phil Biggin (2016)
Secretary	Garrett M. Morris (2017)
Treasurer	Brendan Howlin (2015)
Membership Secretary	Steve Maginn (2016)
Meetings Secretary	—
Journal Editor	Jamie Platts (2016)

Ordinary Members (7)	Val Gillett (2015)
	Jiayun Pang (2015)
	Irina Tikhonova (2015)
	Adrian Mulholland (2016)
	Richard Bryce (2017)
	Stuart Firth-Clark (2017)
	Shozeb Haider (2017)

Co-opted members for 2017-2018 are Louise Birch, Ewa Chudyk, Tim Clark, Ben Cossins, Xiao Lewell, Mike Mazanetz, and Dave Winkler.

9. Any other business

There was no other business.

10. Date and location of next AGM:

The AGM will be held alongside the “Discrete Models in Systems Biology” meeting, at the Møller Center, Churchill College, Cambridge. Provisional date is Wednesday, 29th August, 2018.