



# The Molecular Graphics and Modelling Society

## 38<sup>th</sup> Annual General Meeting

*12:30-2 pm, Monday, 17th June, 2019.*

*Venue: High Tor 3, The Edge, Endcliffe, 34 Endcliffe Crescent, Sheffield. S10 3ED*

*<https://cisrg.shef.ac.uk/shef2019/>*

### *Minutes*

*Present:* Philip Biggin, Garrett M. Morris, Brendan Howlin, Steve Maginn, Val Gillet, Richard Bryce.

**1. Minutes of the 37<sup>th</sup> AGM held at the Murray Edwards College, University of Cambridge, Cambridge, UK**

- The minutes were approved.

**2. Matters arising**

- There were no matters arising.

**3. Chairman's Annual Report**

- PB presented the 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 29-31<sup>st</sup> 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 30<sup>th</sup> 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 30<sup>th</sup> 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 12<sup>th</sup> 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 39<sup>th</sup> 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](http://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 Joint Molecular Graphics and Modelling Society and the Chemical Structure Association Trust's Eighth Joint Sheffield Conference on Chemoinformatics, here at the University of Sheffield, U.K. (17-19 June, 2019), the MGMS has been involved in the organization and support of the following events since the last AGM:

- **Discrete Models and Formal Verification in Biology**, Murray Edwards College, University of Cambridge, U.K. 29-31 August, 2018.
- **Young Modeller's Forum 2018**, University of Greenwich, U.K. 30 November, 2018.
- **“Big Ideas for Big Data” Meeting**, UCL School of Pharmacy, London, U.K. 12 April, 2019.
- **MGMS Lecture Tour** by Dr David Glowacki.

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

Prior to today's elections, the composition of the current committee/trustees is given below (with dates of election in parentheses). Many thanks to all of the committee for their hard work over the year.

<b>Chairman</b>	Phil Biggin (2016)
<b>Secretary</b>	Garrett M. Morris (2017)
<b>Treasurer</b>	Brendan Howlin (2018)
<b>Membership Secretary</b>	Steve Maginn (2016)
<b>Meetings Secretary</b>	—
<b>Journal Editor</b>	Jamie Platts (2016)
<b>Ordinary Members (7)</b>	Richard Bryce (2017)
	Stuart Firth-Clark (2017)
	Shozeb Haider (2017)

	Val Gillett (2018)
	Jiayun Pang (2018)
	Irina Tikhonova (2018)
	Adrian Mulholland (2016)

Co-opted members for the current year were: Louise Birch, Ewa Chudyk, Tim Clark, Ben Cossins, Mike Mazanetz, Michelle A. Sahai, Dave Winkler, and Ian Wall.”

## 5. Treasurer’s Annual Report

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

1) The Meeting on Big Ideas for Big Data which was held on 12 April 2019, School of Pharmacy, UCL, London, U.K.,  
portion of the profits = £5,960.95

2) The first “MGMS Frank Blaney Award”, which was previously known as the MGMS Silver Jubilee Prize, was awarded to Dr Christopher Rowley, the Chemistry Department, Memorial University of Newfoundland, St John’s, Canada.

3) We intend to move our credit card facilities from Barclaycard to CAF Bank, where we have our accounts.

4) Current balances, as of 20/08/18:

Current	£47,526.16	( 2017: £40,454.31)
Savings	£17,016.19	(2017: £17,001.63)

## 6. MGMS Membership and Fees

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

“MGMS membership currently stands at a figure of 268. However, this is following the addition of new members from all meetings up to and including the Big Data meeting in London in April 2019 – and members who joined in 2017 and have not renewed have not yet been removed from the list. This will be done at the end of this month, and will reduce the membership number to 154. The current conference in Sheffield will also provide a considerable boost to our numbers. Conference / meeting attendance remains by far the biggest source of members for the Society.

Regular emailings of items of interest to the membership (relevant job opportunities, relevant non-commercial conference notifications, society news etc.) continue to be sent through a webmail address, [membership@mgms.org](mailto:membership@mgms.org) to members who have consented to receive them; members can opt out of receiving this information at any time..”

## 7. **The Journal of Molecular Graphics and Modelling Society**

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

“Dr Emilio Esposito and myself confirmed as US- and UK-based editors until at least end of 2020.

“Best Graphics” prize named in honour of Jeffrey Madura’s memory, and awarded to Figure 5 in: Multiscale molecular dynamics simulations of lipid interactions with P-glycoprotein in a complex membrane, Domicевичa et al (Vol. 80, 2018, pp. 147-156) Impact factor for 2017 to 1.885 (from 1.754) from 765 submissions and 270 accepted articles (36% acceptance rate). CiteScore for 2018 = 1.92

Over 800 submissions in 2018: current figures suggest further increase in submissions is likely for 2019

Submissions from MGMS members are very welcome! We are also keen to recruit new, motivated members of our Editorial Board: please express any interest to me.”

## 8. **Election of Trustees/Committee Members and Chair**

- Retiring: No-one.
- Re-standing: Phil Biggin, Steve Maginn, Jamie Platts, and Adrian Mulholland.

As no-one stood against those re-standing, everyone re-standing was re-elected.

Following the AGM elections, the MGMS Executive Committee composition is as follows:

<b>Chairman</b>	Phil Biggin (2019)
<b>Secretary</b>	Garrett M. Morris (2017)
<b>Treasurer</b>	Brendan Howlin (2018)
<b>Membership Secretary</b>	Steve Maginn (2019)
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<b>Journal Editor</b>	Jamie Platts (2019)
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	Shozeb Haider (2017)
	Val Gillett (2018)
	Jiayun Pang (2018)
	Irina Tikhonova (2018)
	Adrian Mulholland (2019)

Co-opted members for the current year were: Louise Birch, Ewa Chudyk, Tim Clark, Ben Cossins, Michelle A. Sahai, Dave Winkler, and Ian Wall.

Note: Mike Mazanetz stood down in the last year.

**9. Any other business**

There was no other business.

**10. Date and location of next AGM:**

The AGM will be held at the [\*“Computational Drug Design: A Tribute to Frank Blaney” Meeting\*](#) at [Riddel Hall, Queen’s University, 185 Stranmillis Road, Belfast BT9 5EE](#), on 17 June, 2020, after the last talk of the day.