

The Molecular Graphics and Modelling Society

39th Annual General Meeting

24th November 2020, 2-4.00 pm, via ZOOM after special webinar from Professor
Rebecca Wade

CHAIR'S REPORT

This year has been, to coin an overused phrase, completely unprecedented, due to COVID-19. The pandemic has wreaked havoc on health and economies across the entire globe. Scientific work has been severely interrupted and there is no doubt that it has made our community pause and think about to what extent global travel is needed for scientific engagement and discussion. Indeed, that is why this year's AGM will be held via Zoom. I personally believe that at some point we will return, albeit perhaps to a lesser extent, to in-person conferencing and discussions. We have discovered that the technology for teleconferencing is sophisticated and reliable enough to allow for a good presentation experience. Indeed there are several advantages to this form of engagement not least cost, no physical space limits, and the chance for audience members to ask questions in a different (usually more concise!) way. However, it has also become apparent that the vital informal interactions that occur at physical conferences are not well-reproduced by teleconference/webinars.

Despite the viral backdrop to the latter half of this period, the MGMS continues to be successful in organizing events that achieve its objectives. The first event to report on was the Eighth Joint Sheffield Conference on Chemoinformatics on the 17-19th June 2019 at the University of Sheffield, Sheffield, U.K. This series of meetings first started in 1998 and has continued every three years ever since which reflects its high standing within the community built over the years and the exceptional organizational team behind it. Once again, I would like to extend my gratitude to Val Gillett, Peter Willett, Dave Winkler, Nathan Brown and Garrett Morris for another truly excellent and enjoyable meeting.

Next in the calendar was a joint conference held with CCPBioSim titled "Modelling and Simulation for Synthetic Biology" which was held on the 4th-6th September at the University of Bristol, UK. This was a thoroughly enjoyable meeting that brought together a diverse group of people. An excellent dinner on the SS Great Britain was a particular highlight! My sincere thanks to the organizers of that meeting Marc van der Kamp, Adrian Mulholland, Sarah Harris, Manda Baynes, Ross Anderson and Sarah Fegan.

The final event of 2019 was the "Young Modeller's Forum 2019" held for the fifth time at the University of Greenwich on the 29th November, 2019. Once again, the quality of the presentations both during the talks and the poster sessions was formidable and demonstrates the maturity of the field and the talent within the UK and Europe in this area. The event was 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 and in particular Dr Colin Edge. The support allows us to keep this event free to attend and even to provide some limited travel expenses. The talk winners were Viivi Hirvonen, University of Bristol, Andrew Potterton, UCL and Alistair Sterling, University of Oxford. The poster prizes were awarded to Marius Kausas, The Francis Crick Institute and Kings College London and Stamatiia Zavitsanou, University of Oxford. Congratulations to them all. My particular thanks are extended to Jiayun Pang and Mike Mazanetz, who were once again ably supported by Louise Birch and Steve Maginn. Quite often, the YMF is one of the first events to occur after the AGM. Of course, given the pandemic and the fact that the situation is unlikely to be very different by the end of November, it is currently unlikely, for the first time since its inception, that the YMF will take place physically. However, at least some of this format (the talks) could be done as a one-day webinar and we are currently discussing how that might proceed. I think it is particularly important that we try to make this work as presenting opportunities for younger scientists are rather thin on the ground at the moment.

Before the lockdown kicked in, the very first MGMS Early Career Workshop Initiative was held at Imperial College in February with the title “Modeling Photoinduced Processes in Molecular Systems” and organized by Javier Segarra Marti and Lara Martinez. The MGMS Early Career Workshop Initiative 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. Another call for this will be made later this year once we have a better idea of how the pandemic is developing.

The sponsorship of prizes is another important way in which the Society seeks to promote computational chemistry. This year, the second “*MGMS Frank Blaney Award*” was awarded to Isidro Cortes-Ciriano of the European Bioinformatics Institute (EMBL-EBI). His work is focused on the development and use of computational methods to characterize the patterns of mutations and genome instability processes in human cancers. Congratulations Isidro! 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 call for nominations for the 2020 Award only just recently closed and there were several high quality submissions. Results for that will be announced shortly.

This year, the *MGMS Lecture Tour* was given virtually by Professor Rebecca Wade, of the Heidelberg Institute for Theoretical Studies, later this year. My thanks to Rebecca for so readily agreeing to do this virtually. Of course, plans for next years “Tour” are on hold until we know about how the pandemic situation will evolve. However, if you have an idea for someone who you would like to see undertake such a Tour either virtually (in the near future) or physically (in the farther future!) then please do not hesitate to get in touch.

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 40th 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. This year will be challenging but I am sure we can continue to make a strong impact and support our community through these strange and disconcerting times.

Philip Biggin, Chair of the MGMS

November 2020