

The Molecular Graphics and Modelling Society

40th Annual General Meeting

24th September 2021, 5.30 pm, via ZOOM after “MGMS at 40”

CHAIR’S REPORT

This year is a rather special year for the MGMS – it is 40 years old and thus celebrating its Ruby Anniversary! Unfortunately, the continuing restrictions of the pandemic has meant that we have had a relatively quiet year in terms of conferences and events. Although the reliability and quality of the technology now available for tele/remote conferencing has proven robustness, a new phenomenon arose – “Zoom fatigue”! The upshot was that the most popular format for remote conferences was a ½ day zoom meeting and those generally appeared to have worked quite well as hopefully today’s event will testify. The uncertainty over the pandemic and the potential restrictions on in-person gatherings means that we are likely to have to tread carefully in terms of making commitments in the coming year with future conferences. Nevertheless, the high vaccination rates within the UK and the relaxation of restrictions give hope that possibly at some point in the coming year we may be able to run a small in person event. In-person events are particularly important for younger scientists, where interaction and informal advice can be incredibly valuable at the start of one’s career.

Last year, the disruption of the pandemic meant that we were, for as long as I can remember, unable to hold the Young Modeller’s Forum (YMF) as an in-person event in November. Instead, and as anticipated in my last report in fact, it was held as an online event over zoom on the 12th February 2021. The event was a great success, and all the presenters were unphased by the move to an online platform, with all of them delivering excellent high-quality talks and posters. My thanks once again to Jiayun Pang, Louise Birch and Steven Maginn for their hard work in making this event a success. The 2021 YMF is due to take place at the end of November, and whilst it may yet be possible to run this as an in-person event, it would seem likely that for another year at least, we will have to use the online forum. Online does mean however, that we can vastly expand the number of attendees, but for presenters the experience can feel relatively flat. As ever with these things, it’s swings and roundabouts.

The only other event to report on, was an event that the MGMS was very proud to be part of and support – the “underrepresented groups and allies in computational chemistry meeting” operating with the strap line “Being #CompChemURG: How Diversity Enriches Us”. This event was organized by Michelle Sahai and Hannah Bruce-Macdonald and the focus was to show the diversity amongst the comp-chem community and highlight some of the issues and challenges that are often faced. It was an incredibly inspiring event and my deepest thanks to both Michelle and Hannah for taking it on as well as the Royal Society of Chemistry for providing some financial support.

The sponsorship of prizes continues to be a key way that the Society seeks to promote computational chemistry. This year, the third “MGMS Frank Blaney Award” was awarded to Fernanda Duarte-Gonzalez of the University of Oxford. Her work is focused on the development and use of computational methods to investigate organic chemistry. Congratulations Fernanda! 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 2021 Award is open, and the deadline is the 5th November 2021, so get your nomination in! Results for that will be announced shortly thereafter.

The MGMS Lecture Tour is currently on hold in the physical sense. However, if you have an idea for someone who you would like to see undertake such a Tour virtually or indeed physically (when travel becomes easier) 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 Ewa Chudyk 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 his continuing role as webmaster.

As the Society enters its 41st year, which is no mean feat for a charity run by volunteers, I am sure that the MGMS will continue to make an important impact in promoting all avenues of computational chemistry through the various meetings, lectures, prizes 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. We are always happy to co-opt members onto the committee so don’t be shy!

This year will again be rather unusual in terms of activities, but we have adapted well, and I am sure will continue to help and support the next generation of computational chemists and biochemists.

Philip Biggin, Chair of the MGMS

September 2021