

The Molecular Graphics and Modelling Society
33rd Annual General Meeting

20th August 2014, 3:45-4:30pm, McCance building (Main Lecture Theatre), The University of Strathclyde, MGMS M3 Conference.

CHAIR'S REPORT

The Molecular Graphics and Modelling Society is a charitable society whose aim is to promote education and research into molecular graphics and modelling. One of the main ways this is achieved is through the organisation of meetings by its volunteers, such as this current "Modelling Molecules and Materials" meeting at the University of Strathclyde. Our thanks go to David Cheung, Hans Martin Senn and Tell Tuttle for their hard work in putting together an excellent and wide ranging scientific programme.

I am pleased to report another active and full year for the Society, which began last July with the triennial Sheffield Conference on Cheminformatics, organised jointly with the Chemical Structures Association Trust. Later in the year, there was a meeting on "Cytochrome P450s: Modelling Toxicity" at the University of Surrey. In January, there was a meeting on "Multiscale Modelling of Condensed Phase and Biological Systems" in Manchester, organised jointly with CCP-BioSim and CCP5. In coordination with this meeting, the Society sponsored the visit to the UK of Professor Adrian Elcock of Iowa University, as an MGMS Tour Lecturer. Prof Elcock, an expert in modelling of macromolecular crowding effects, gave a plenary talk at the Manchester meeting and was hosted at Leeds, Oxford and UCL. In March, there was a one-day meeting in London on Cutting Edge Approaches to Drug Design, profiling the state-of-the-art in modelling the influence of water on biological systems. In May, the MGMS was a cosponsor of the RSC Faraday Discussion entitled "Molecular Simulations and Visualization", a meeting whose theme chimed with the molecular graphics roots of the Society. The MGMS sponsored a second Lecture Tour, this time by Professor Art Olson, who gave illuminating presentations at the Discussion and other UK venues (Cardiff, Oxford, Cambridge and GSK).

The annual Young Modellers Forum provided its usual excellent showcase of talented modellers, profiling the work of postgraduate computational chemists and biologists. There was strong competition for the coveted 12 poster and 12 oral presentation places. The names of the winners for the best oral and poster presentations can be found on the MGMS website.

The sponsorship of prizes is another important way in which the Society seeks to promote computational chemistry. The prestigious MGMS Silver Jubilee Prize is awarded each year to outstanding young researchers in the field. Competition for this prize is fierce, attracting international nominations of the highest calibre. This year, the 2014 prize was awarded to Dr Robert Paton from the University of Oxford, for his work on computational modelling of structure, reactivity and selectivity in organic and bioorganic chemistry. We congratulate him and look forward to the continued success of the prize.

As the past year has been another active one for the MGMS, there is much to look forward to in the year ahead including the YMF on the 28 November in London and a three-day meeting on "Membrane Signalling and Transport: Computation and Experiment" at the University of Oxford (15-17 April). The success of these activities, which play a vital role in promoting computational chemistry and the cohesiveness of its 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. At this meeting, Charlie Laughton and Richard Ward have chosen to stand down as members of the committee. I would like to thank them both for their contributions to the MGMS over the past years. This is also my final report as Chair. I would like to thank all the committee for their commitment and enthusiasm and support over these last three years. My particular thanks go to Richard Ward and Phil Biggin for their hard work as Secretary and Treasurer respectively. Phil has also agreed to stand as Chair of MGMS, a role in which I am sure he will do an excellent job and for which he has my full support. The Society also owes a debt of thanks to Jonathan Hirst for his hard work as Editor of the Journal of Molecular Graphics and Modelling over the last nine years, a time which has overseen further growth in the journal's reputation. I am pleased to announce that Jamie Platts from Cardiff University will take the helm as Editor from the end of the year.

As the Society enters its 34th 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 around meetings that you would like to see and get involved with, then please do contact myself or other committee members.

Richard Bryce

Aug 2014