Computational Molecular Science meeting – CCP9 Report

Title, Location, and date of meeting:
The 6th Computational Molecular Meeting (CMS), held at the University of Warwick from March 26th to March 29th.

Name of organizers:
Dr. Gabriele C. Sosso (g.sosso@warwick.ac.uk | https://www.sossogroup.uk | @SossoGroup) and Dr. Reinhard J. Maurer (r.maurer@warwick.ac.uk | https://warwick.ac.uk/fac/sci/chemistry/research/maurer/maurergroup/ | @reinimau)

Number of participants:
155 – including organisers and speakers.

Aim of event:
To take stock of the latest advances in the diverse field of computational molecular science. The meeting featured five session: (1.) Biomolecular Simulations, (2.) Energy Materials and Interfaces, (3.) Density Functional Theory - Methods and Applications, (4.) Advanced Quantum Chemistry and (5.) Machine Learning. We tailored the programme in such a way to highlight the future challenges for the community.

Major outcomes
- *Biomolecular Simulations:* Multiscale modelling, including QM/MM approaches, is paving the way to strong connections with the experimental reality. We have a real opportunity to provide qualitative insight into countless biomolecular systems – but we need to make sure our data is backed up by proper statistical analysis and uncertainty quantification.
- *Energy Materials and Interfaces:* There is a genuine drive toward adding layer upon layer of complexity in simulations of energy materials and heterogenous systems – with a clear need for further methodological developments.
- *Density Functional Theory - Methods and Applications*: The debate on exchange-correlation functionals (not just about *which* ones should we favour/use, but also whether we need some more) is still very much unfolding, with many research groups seeking cross-validation with either experiments or alternative computational methods.
- *Advanced Quantum Chemistry:* We have reached the point where extremely accurate calculations can take into account systems far more complex/big than the "usual" H_2 molecule. A number of recent developments from junior group leaders has to be noted/commended as a brave choice to get back to the basics.
- *Machine Learning:* Machine learning is rapidly becoming ubiquitous – about 80% of the poster contributions contained the "machine learning" keyword in some form. How to navigate the hype was a hotly debated issue. While we recognize the dangers in riding the tide, we are also constrained by the requirements of the current funding landscape, in the UK especially.

Impact
The meeting was very well received, and especially impactful in mainly two different aspects: (1.) it enabled the rare cross-fertilization between very different fields (e.g. biomolecular simulations and advanced quantum chemistry) and (2.) allowed us to pinpoint a number of key challenges for the community to tackle in the next few years.

Conclusions
This was the 6th establishment of the CMS meeting: in two years' time we anticipate a change of venue, possibly steered by a steering committee we are working to build as we speak. While it is impossible to summarise the outcomes of such a multifaceted event, we can safely say that it was a phenomenal opportunity to showcase young talents and bring them together with absolute legends: we have high expectations for the CMS 2021.