

Molecular Spectroscopy Science Meeting – MSSM2018

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The latest edition of the *Molecular Spectroscopy Science Meeting (MSSM2018)* took us to the Christopher Ingold Building at University College London (UCL), home to its thriving and busy Department of Chemistry. Held on 6-7th November 2018, we enjoyed the attendance of over seventy participants from the United Kingdom and beyond.

This year, focus was placed on industrial challenges and how neutron spectroscopy is being used to tackle these from a variety of perspectives. To this end, two back-to-back thematic sessions focusing on both experimental and computational work kicked off the event in the early afternoon of the first day. These were followed by three thematic sessions: *Back to Fundamentals – Water & Aqueous Media*, also during the first day; as well as *Environmental Materials* and *Looking Back – Archeometry & Cultural Heritage* during the second and final day. To stimulate further discussion, presentations by Stewart Parker, Sanghamitra Mukhopadhyay, Franz Demmel, and Matthew Krzystyniak served to wrap up each of these sessions, highlighting the most recent updates from the *Molecular Spectroscopy Group* since our previous gathering in 2016. For the first time, these presentations were also supplemented by a MANTID surgery held throughout the meeting, an opportunity to gather feedback for the further development of data-analysis and in-silico tools.

The meeting was officially opened by Stephen Price (UCL Chemistry) as our host, regaling us with an overview of current research in the department, as well as snapshots of the history of the Bloomsbury campus and some of its most celebrated dramatis personae, including the legendary Jeremy Bentham. This welcome address was followed by introductory remarks by Christoph Salzmann (User Group Chair, UCL) and Felix Fernandez-Alonso (Head of the Molecular Spectroscopy Group, ISIS & UCL) in order to set the aims and scope of the meeting, in many respects quite different from previous editions. These initial moments were also an opportunity for Christoph to hand over his responsibilities as User Group Chair to Roberto Senesi (Università di Roma – Tor Vergata), as well as to welcome nominations for a User Group Representative to join the team.

The first thematic session of the day on *Industrial Challenges* started with an invited talk by Alexander de Bruin (Johnson Matthey) on the use of low-energy neutron spectroscopy to look at automotive catalysts, a joint venture involving the flourishing UK Catalysis Hub and currently focused on OSIRIS for concurrent structural and spectroscopic studies. Andrea Zachariou (Glasgow) then explained the conversion of methanol to hydrocarbons in zeolite catalysts, a superb example of the chemistry that is currently possible around a growing number of neutron instruments including TOSCA, MAPS, or MERLIN. And Guillaume Schweicher from Cambridge presented exciting results on how electron-phonon coupling can be used to design new materials for electronics, clearly capitalising from the recent guide upgrade of TOSCA.

Angelos Michalides (UCL) opened the second part of our *Industrial Challenges* session with a comprehensive overview of computational studies at interfaces, including current limitations of density-

functional-theory approaches to predict adsorption energetics, as well as subtle yet at the same time significant nuclear quantum effects. Pierfrancesco Ulpiani (Tor Vergata) shifted gears during a second talk devoted to new developments in epithermal-neutron instrumentation, with a focus on the current incarnation of VESUVIO and further opportunities for its successor ETNA. Keith Butler (ISIS) then presented fresh results on structure-property relationships in lead-halide perovskites for photovoltaic applications, tackled via a judicious combination of experimental and computational efforts capitalising from recent instrumentation and in-silico developments within the MANTID framework.

The latter part of the first afternoon took us *Back to Fundamentals*, with an emphasis on water and aqueous media. Paul McMillan (UCL) explained how quasielastic neutron scattering has been used to address the challenging goal of probing the state of water in bacteria at high pressures, with recent results from a variety of high-resolution instrumentation across Europe including IRIS. Silvia Imberti from ISIS updated us on recent efforts to understand co-nonsolvency at the molecular level, with a view to exploring how spectroscopy may be used in conjunction with total-scattering techniques. And Ciprian Pruteanu (UCL) concluded this final scientific session of the first day by showing how oil and water can mix, a very counterintuitive phenomenon entirely driven by pressure.

As the day came to a close, the UCL South Cloisters witnessed our traditional 'gong-driven session' of one-minute poster presentations. Competition for the poster prize was at an all-time-high, with over 20 contestants delivering a rapid set of brief and well-articulated 'spiels,' prior to a more relaxed poster session around nibbles and drinks and a subsequent dinner at the Jeremy Bentham Room. This year's poster prize went to Barbara Souza from Oxford University, for her work on guest-host interactions in anti-cancer drugs encapsulated in metal-organic frameworks (see figure below). Adriana Mamede (Coimbra) and Joel Ponsonby (ISIS) were also amongst the best three posters presented, 'nanometers away' from the prize.

Environmental Materials greeted us early in the morning of the second day, with Neal Skipper (UCL) telling us about the prospects of using natural and synthetic clays for gas storage and sequestration. Mi Tian (Bath) continued along similar lines using microporous carbons, including yet-to-be-explained isotope effects in the adsorption of molecular hydrogen in these materials. Kun Tian from Tor Vergata took us to the world of clinical dentistry, with intriguing yet at the same time useful correlations between mechanical properties and atomic cohesion.

The last session of the meeting focused on an emerging and growing area, *Archeometry & Cultural Heritage*. Maria Paula Marques (Coimbra) described how high-resolution broadband neutron spectroscopy on burned bones can talk to us about ancient civilisations. Claudia Scatigno (Tor Vergata) explained the use of modern chemometric tools to analyse parametric data from high-throughput spectroscopic studies on the new TOSCA. And Laura Arcidiacono (Tor Vergata and UCL) described the recent implementation of time-resolved prompt-gamma-activation techniques for a variety of applications including archeometry – a superb and timely example of the merits and strengths of pulsed neutrons. A final discussion summarising the event and calling for further discussion and input from the floor was led by our new User Group Chair Roberto Senesi.

In closing this brief summary, we can't thank all attendees and participating institutions enough for a very enjoyable and productive meeting, showcasing a number of areas and opportunities unthinkable not so long ago, from real-life applications in partnership with industry to the development of new and ingenious ways of doing neutron spectroscopy. If you could not make it this time around, please come along next time, venue still to be decided!



MSSM2018 attendees posing at the entrance of the Ingold Building at UCL (Reproduced with permission of Jonathan Oldfield, Science & Technology Facilities Council).



Poster prize winner Barbara Souza presenting her work during our 'one-minute gong session' at the UCL South Cloisters (Reproduced with permission of Jonathan Oldfield, Science & Technology Facilities Council).