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Guest Editorial

Advanced Characterisation and the Net Zero Transition

Net zero is the topic that will dominate the political, and hence the industrial, landscape for decades to come. As of 23rd April 2021, 44 countries (including the UK) and the European Union have pledged to meet net zero (1). Together, these countries are responsible for ~70% of global CO_2 emissions and gross domestic product (GDP).

For net zero to be achievable, chemistry will have to play a major role (2). In 2016, chemical manufacturing accounted for 5.8% of global greenhouse emissions. Transport was responsible for 16.2% of emissions, as transportation is dominated by products from the petrochemical industry, in total, the chemical industry accounts for 22% of global greenhouse emissions (10.9 billion tonnes CO_2 eq.) (3). As more than 80% of chemical processes involve catalysis at some stage (2), it is apparent that catalysis, and the study of catalysts, will be an absolutely essential component in the successful implementation of net zero.

The Role of Characterisation in Net Zero

Characterisation lies at the heart of materials science and particularly so for catalytic science. The need for characterisation spans fundamental science ("what have we made?") to industrial products ("does it meet the specification?"). As catalysts and related materials have become more complex, so the need for characterisation has grown. While a simple statement about the composition of a catalyst, for example Pt(10 wt%)/C, may have been sufficient in the past, today, the particle size distribution, morphology and the interaction between the metal particle and the support are increasingly expected to be provided. There is also a huge effort made to understand the mechanism that underpins a

reaction or process. The result of the need for better characterisation at all levels from the atomic to the macroscopic has been a relentless drive to develop ever more sophisticated tools that can address these questions.

Next Generation of Techniques

The next two issues of this journal feature 11 themed papers that showcase techniques at the very edge of current capabilities. They are used to investigate problems as diverse as understanding materials derived from renewable sources (4–7), solid oxide fuel cell catalysts (8), zeolite catalysis (9–11), structural studies of alumina (12) and the migration (13) and particle size changes of working catalysts (14).

Central facilities provide access to techniques that are either not possible in a laboratory, for example neutron scattering, or are severely constrained, such as laboratory X-ray sources as compared to synchrotron X-rays. The STFC Rutherford Appleton Laboratory at Harwell, UK, exemplifies this capability as it hosts the ISIS Neutron and Muon Source (ISIS), the Diamond Light Source (DLS, a third generation synchrotron) and the Central Laser Facility (CLF). Four of the papers in this theme (9–11, 14) make use of these facilities to understand materials at the atomic and molecular scale.

I would like to highlight two papers that clearly show how the characterisation of materials is changing and point the way to the next generation of techniques. The first of these is the work by Cavaye and Schuster (14) that used machine learning (ML) to analyse electron microscopy images. It is likely that the use of artificial intelligence (AI) and ML will become an integral part of analytical chemistry, particularly where large datasets are generated.

The second paper is the article by Donaldson et al. (11) that describes a range of laser-based spectroscopies. This field is advancing very rapidly driven by the introduction of femtosecond lasers. Two notable developments are Kerr-gated Raman spectroscopy and two-dimensional infrared spectroscopy (2D-IR). The first of these enables fluorescence-free Raman spectra to be obtained from catalysts. While Raman spectroscopy has long been used to study catalysts (15), generally it fails because of fluorescence. This technique provides a near universal solution to the problem of fluorescence and has already enabled operando methanol-to-hydrocarbons studies of the reaction using H-ZSM-5 (16). 2D-IR can be used to investigate how modes are coupled to gain insight into the species present. Both of these developments are likely to feature strongly in catalytic science over the next decade.

Finally, the geographic spread of the papers is noteworthy. Approximately half of the authors are from Europe and the USA, the remainder are from India and south-east Asia. This reflects the diversity present in catalytic science and bodes well for the future.

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