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Computational modelling in catalytic science

C. Richard A. Catlow, *[abc] Arunabhiram Chutia *[d] and Matthew G. Quesne *[bc]

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Catalytic science poses fascinating fundamental challenges while being of major industrial and societal importance. Moreover, responding to the fundamental scientific problems is vital in optimising and designing catalysts with improved efficiency and novel functionalities. The field has been transformed in recent decades by the development and application of advanced analytical and characterisation techniques, both experimental and computational. Indeed, recent themed issues of this journal have highlighted the role which **neutron scattering** and **synchrotron radiation** based techniques are playing in the field. In this issue, we focus on the growing role of computational modelling at the atomic and molecular level which is now contributing to almost all aspects of both fundamental and increasingly applied catalytic science.

The collection shows the breadth of current computational catalytic science with all branches of the field – hetero-, homo- and biocatalysis – being well represented. It also highlights some of the key current application areas. Well-represented themes include novel chemical routes for important challenges in environmental and energy science, including: the efficient conversion of greenhouse gases, the removal of water pollutants, ammonia synthesis, the upgrading of biofuels and the electrocatalytic splitting of water.

The growing focus on the fine-structure, morphology, and support interactions of various heterogeneous catalysts is reflected in the collection. Importantly, there are a diverse array of changes reported in catalytic properties when these effects are included explicitly in computational models. The growing predictive power of computational modelling in catalysis is also highlighted by articles describing the design of new and more efficient heterogeneous and biocatalytic routes that are as yet not confirmed experimentally.

The range of methods described in this collection is also very wide and diverse. However, a constantly reoccurring theme is the need for truly multi-scale and multi-method approaches to many catalytic problems. Several studies report the effectiveness of combining sampling techniques or machine learning to achieve more accurate electronic structure calculations techniques. Prominence is given to the latest developments in the multiscale implementation of hybrid QM/MM (quantum mechanics/molecular mechanics) techniques to various heterogeneous and biocatalytic reactions, as well as exemplar studies that highlight the effectiveness of a combination of density functional cluster models and QM/MM techniques in rationalising the catalytic activity of enzymes.

The collection additionally signposts important new toolkits for catalytic modelling, with sources for multiscale tutorials and new codes for quick evaluation of metal/adsorbate interactions presented, which is combined with a careful evaluation of many of the limitations of current methodologies, and with a focus on future developments to improve the accuracy of current techniques.

Articles revisit well-established catalysts, examining previously overlooked electronic and structural properties, such as, the activity and or product selectivity of higher energy facets, the identification of previously unreported active spin-states as well as the effects of nanoparticle size and their support interactions, highlighted earlier. The importance of data driven approaches to reduce the chemical space of potential catalysts is discussed in several studies. Finally, there is the commonly occurring theme of electronic and electrostatic effects of catalyst components often far removed from the active site region, which is known often to be important in biocatalysis but which also can be significant in other areas of catalytic science.

[a] *Department of Chemistry, University College London, 20 Gordon St, London WC1H 0AJ, UK. E-mail: c.r.a.catlow@ucl.ck.uk*
[b] *UK Catalysis Hub, Research Complex at Harwell, Rutherford Appleton Laboratory, Harwell Oxford, Didcot OX11 0FA, UK*
[c] *School of Chemistry, Cardiff University, Park Place Cardiff, CF10 3AT, UK. E-mail: quesnem@cardiff.ac.uk*
[d] *School of Chemistry, Joseph Bank Laboratories, Brayford Pool, Lincoln University, Lincoln, LN6 7DL, UK. E-mail: achutia@lincoln.ac.uk*

Computational modelling in catalytic science is a fast developing field, benefitting from developments in techniques, algorithms and hardware; and it is clear from this collection both that the pace of advancement is set to increase, and that the predictive power of the field and its increasing integration with experiment will grow. No single volume can cover the field; however, we hope that this collection offers an overview of the current state-of-the-art, as well as highlighting some of the most important new resources and approaches for computational catalytic research.

