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The Synergy between Theory and Experiment

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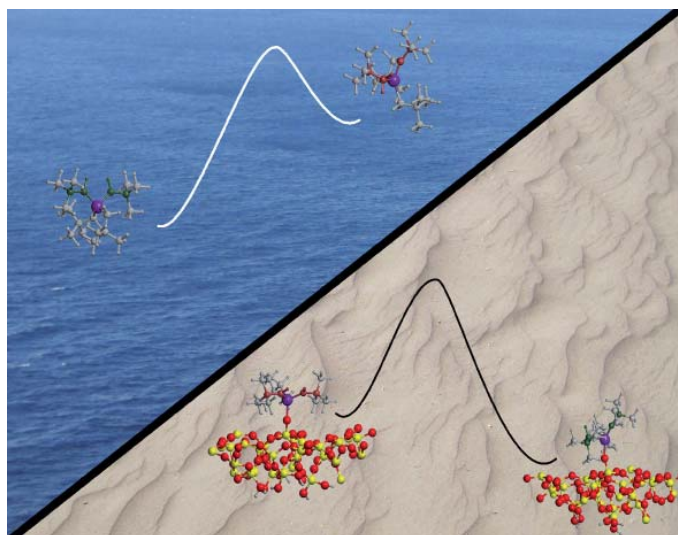


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Papers published in this issue include:

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Per E. M. Siegbahn and Margareta R. A. Blomberg, *Dalton Trans.*, 2009,
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Youssef Boutadla, David L. Davies, Stuart A. Macgregor and Amalia I. Poblador-Bahamonde,
Dalton Trans., 2009,
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Malcolm H. Chisholm and Namrata Singh, *Dalton Trans.*, 2009
DOI: [10.1039/b901734h](#)

[Molecular recognition in Mn-catalyzed C–H oxidation. Reaction mechanism and origin of selectivity from a DFT perspective](#)

David Balcells, Pamela Moles, James D. Blakemore, Christophe Raynaud, Gary W. Brudvig, Robert H. Crabtree and Odile Eisenstein, *Dalton Trans.*, 2009
DOI: [10.1039/b905317d](#)

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The synergy between theory and experiment

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Welcome to this themed issue of *Dalton Transactions* entitled 'The synergy between theory and experiment'. The aim of the issue is to highlight the close relationship between experiment and theory that underpins much of modern inorganic chemistry. The dramatic advances that theoretical inorganic chemistry has made are neatly illustrated by taking snapshots from the pages of this journal over the past 25 years. Up until the early 80s, theoretical contributions to inorganic chemistry relied heavily on methods such as extended Hückel theory. The inability to compute accurate total energies using such tools was both a limitation and (at least in some senses) a blessing, because it forced practitioners to think very carefully about the links between their calculations and experimental observations that had motivated them. The profound influence of the

work of Nobel Laureate Roald Hoffmann on a generation of chemists is testament to the power of such qualitative arguments. A decade on and these simple models were largely being supplanted by density functional theory, where the availability of total energies, alongside the development of effective algorithms for locating stationary points, opened the door to analysis of potential energy surfaces. As a result, theory began to make significant contributions to our understanding of inorganic reaction mechanisms and catalysis. Fast forward to the present day and the number of papers containing some element of theory has increased dramatically, with applications in spectroscopy as well as structure and mechanism now commonplace. Perhaps more importantly, there has been a distinct change in the way in which theory and experiment are integrated: whilst in the past

papers could often be classified as 'experimental' or 'theoretical', fewer and fewer papers now fall neatly into either category. It is more common for the two perspectives to be published alongside each other in the same paper, clearly reflecting the way that one has influenced the other. The current issue celebrates this synergy by bringing together articles dealing with problems in structure, mechanism, spectroscopy and magnetism. The predominance of density functional theory reflects its position at the centre of computational inorganic chemistry, but there are also notable examples involving wavefunction-based methods. I hope that it will provide the reader with an appreciation of how theory and experiment can combine to enhance our understanding of inorganic chemistry.

Professor John McGrady