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Catalysis For Sustainable Chemicals and Fuels

Achieving sustainability is possibly the greatest global challenge of the 21st Century; and developments in catalytic science will be crucial in meeting this challenge. This lecture will explore how a powerful combination of computational and experimental techniques is providing detailed structural and mechanistic insight into a range of catalytic processes of key importance for the development of sustainable chemicals and fuels. Our discussion will concentrate on the following systems:

(i) The mechanisms of CO and CO_2 conversion into methanol over copper and zinc oxide supported copper catalysts.
(ii) The catalytic chemistry of methanol to gasoline conversion in microporous catalysts.
(iii) The dynamics of adsorbed molecules in zeolite catalysts.
(iv) Catalytic ammonia synthesis and the development of new catalytic technologies

We will highlight the role of computational modelling but also show how modelling can be used synergistically with experimental techniques.

Professor Sir Richard Catlow is developing and applying computer models to solid state and materials chemistry — areas of chemistry that investigate the synthesis, structure and properties of materials in the solid phase. By combining his powerful computational methods with experiments, Richard has made considerable contributions to areas as diverse as catalysis and mineralogy.

His approach has also advanced our understanding of how defects — missing or extra atoms — in the structure of solids can result in non-stoichiometric compounds. Such compounds have special electrical or chemical properties since their contributing elements are present in slightly different proportions to those predicted by chemical formula.

Richard's work has offered insight into mechanisms of industrial catalysts, especially involving microporous materials and metal oxides. In structural chemistry and mineralogy. Simulation methods are now routinely used to predict the structures of complex solids and silicates, respectively, thanks to Richard's demonstrations of their power.