

CCST Seminar:

- › Friday, May 22, 2009
- › 11:00 A.M.
- › 366 Colburn Laboratory

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“Simple and Complex Oxides in Selective Oxidation Reactions”

The oxidation of unfunctionalized alkanes is a critical step to produce all monomers for chemical industry in the near and distant future when oil-based processes are no longer feasible. Today, these reactions are in some cases not possible and in some cases operate with poor yields leading to enormous wastes of chemicals and energy and respective carbon footprints.

A common origin of these shortcomings is our lack of ability to control the reactivity of oxygen in the presence of hard-to-activate substrates. In addition, in all relevant reactions the products are thermodynamically less stable than the educts posing additional constraints on the reactivity of the catalyst.

Besides possible novel designs of catalytic reactors enabling a more even profile of the chemical potential throughout the active mass, it is most relevant to understand without critical simplifications the mode of operation of the catalyst. At present, we operate with a set of empirical rules referred to as “pillars of selective oxidation” that lack, however, physical foundation.

In this context, it turns out that simple oxides such as vanadia or complex oxides, such as MoVWNbTeO_x, are not discriminated in their accessibility to the functional part of their surface. All of these catalysts provide enormous challenges in synthesis, operation and functional characterization. The support of surface science models is very useful but limited as they do not provide the necessary functionality when they are well ordered in their structure.

It will be demonstrated that a concept of adaptive sites being part of a cluster-like surface termination of active materials can provide a unified structural concept towards understanding selective oxidation. After all, most of these reactions are a combination of C-H activation and oxygen transfer for which similar elementary steps should operate. This concept was derived from a synopsis of model studies and in-situ functional analysis. The role of solid-state chemistry driving the expression of the active sites under reaction conditions will be highlighted.