

Departments of Chemistry / Physics /  
Institute of Computational and Theoretical Studies

*Joint Colloquium*

*Structural Analysis of Silica-Supported Transition Metal Oxide  
Catalysts by X-ray Absorption: Theoretical cluster studies*



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- Scientific Activities
  - \* Published 3 books on Surface Structure, 3 conference proceedings books
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  - \* 2 Scientific films, 8 Software packages

**Date: 23 January 2013 (Wednesday) Time: 3:00 p.m. – 4:00 p.m.**

**Venue: Lecture Theatre WLB 109, Wing Lung Bank Building  
Shaw Campus, HKBU, Kowloon Tong**

Abstract. Modern theoretical methods applying density-functional theory (DFT) can be used to interpret experimental results from electron spectroscopy, such as X-ray absorption (XAS/NEXAFS) or X-ray photoemission (XPS), and can provide an understanding of structure on a microscopic scale. This talk reviews recent theoretical work on electronic and structural properties of different vanadia-, molybdena-, and titania-silica particles which can form active centers in catalysts of industrial relevance.

DFT calculations, using the StoBe code [1], are performed on oxygen core excitations in different vanadia-, molybdena-, and titania-silica clusters. These results are compared with O K-edge NEXAFS measurements of corresponding catalysts on SBA-15 silica yielding structural details of the nanoparticles. Differently binding oxygen, inside MeOx (Me = V, Mo, Ti) and SiO<sub>2</sub>, can be clearly distinguished in the theoretical spectra. A comparison with experimental NEXAFS spectra for different vanadia species provides clear evidence that polymeric VO<sub>x</sub> exists at the catalyst surface and the exclusive presence of monomeric vanadia groups can be ruled out [2]. Further, the comparison for molybdena species indicates that tetrahedral dioxo MoO<sub>4</sub> units, binding by one or two Mo-O-Si bridges with the silica support, dominate the experimental spectrum [3]. Finally, the comparison suggests that monomeric titania species at low coverage on SBA-15 will form tetrahedral complexes where titanyl oxygen is saturated by hydrogen yielding OH groups at the Ti centers [4].

[1] K. Hermann (FHI Berlin) and L.G.M. Pettersson (Univ. Stockholm + deMon developers community), <http://www.fhi-berlin.mpg.de/KHsoftware/StoBe/index.html>.

[2] M. Cavalleri, K. Hermann, A. Knop-Gericke, M. Hävecker, R. Herbert, C. Hess, A. Oesterreich, J. Döbler, and R. Schlögl, *J. Catal.* 262, 215 (2009).

[3] C.S. Guo, K. Hermann, M. Hävecker, L.J. Gregoriades, J. Sauer, A. Trunschke, and R. Schlögl, *J. Phys. Chem. C* 115, 15449 (2011).

[4] C.S. Guo, K. Hermann, M. Hävecker, A. Trunschke und R. Schlögl, *J. Phys. Chem. C* 116, 22449 (2012).