The Impact of in situ X-ray Absorption Spectroscopy on Heterogeneous Catalysis

Simon R. Bare UOP LLC Des Plaines, IL 60017, USA <u>simon.bare@uop.com</u>

The modern advent of X-ray absorption spectroscopy (XAFS) began in 1971 with the publication of the pioneering paper by Sayers, Stern and Lytle¹. It was only three years later that the first XAFS paper was published that mentioned catalysis². In the last ten years there have been an average of 330 papers published per year that mention "XAFS and Catalysis", with approximately 20% of these conducted under *in situ* conditions. Among the reasons why the technique has found such a wide application to the characterization of heterogeneous catalysts are: it provides element-specific information on the local electronic and geometric structure of the surrounding the element under study. Moreover, these properties can be determined in situ, with the catalyst in the working state. So, what has all this research provided to the field of catalysis? What have we learned? In this talk I will present my personal view of the impact that this body of work has had on our understanding of heterogeneous catalysis, with particular emphasis that the spectroscopy has had on UOP's research. The overall goal of this work is to identify the precise atomic level detail of the catalytically active site, under operating conditions, and understand how the specific details of the catalyst preparation and catalyst activation affect the site, and moreover how different operating conditions affect the site. The assumption is that if we can identify this site, and understand the factors that affect it, then we can design from the ground up a better catalyst with improved performance. This is the so-called "structure-reactivity" relationship. These ideas will be explored using examples primarily from my own research, and also from the vast published body of work in this area.

References

^{1.} D. Sayers, E. Stern, F. Lytle, Phys. Rev. Lett. 27 (1971) 1204

^{2.} F. Lytle, D. Sayers, E. Moore, Appl. Phys. Lett. 24 (1974) 45.