Workshop on Ambient Pressure X-ray Photoelectron Spectroscopy, October 4-5, 2007, Berkeley, CA

Hendrik Bluhm, B. Simon Mun, Miquel Salmeron

Lawrence Berkeley National Laboratory,Berkeley, CA 94720

This workshop focussed on the application of ambient pressure X-ray photoelectron spectroscopy (APXPS) to environmental science and catalysis. Pioneering work on APXPS was done in the early 1970's by Hans and Kai Siegbahn et al., who demonstrated that XPS can operate at pressures of up to 1 Torr. A new type of APXPS instrument that utilizes a differentially-pumped electrostatic lens system at the ALS in 2001 increased the pressure limit to above 5 Torr, which opened the door to XPS experiments on water and aqueous solutions at temperatures above the melting point, in equilibrium with the vapor pressure of water. The impact of APXPS on fields such as environmental and atmospheric science as well as heterogeneous catalysis is already visible in numerous high impact publications. Today several other synchrotron facilities around the world have already implemented beam lines for APXPS or planning to do so in the near future. The goal of this workshop (organized by Miquel Salmeron (Molecular Foundry, LBNL), B. Simon Mun (Advanced Light Source, LBNL) and Hendrik Bluhm (Chemical Sciences Division, LBNL)) was to bring together researchers interested in the technique, review its current progress, discuss scientific opportunities and desirable technical improvements as well as consider the consequences of the increased user demand on the existing beam lines and ways to expand the availability of time. The workshop was attended by about 50 participants.

The workshop was opened by Miquel Salmeron with an introduction into the history and current challenges of APXPS. This introduction was followed by Robert Schlögl (Fritz Haber Institut, Berlin) who in his plenary talk discussed the application of APXPS to heterogeneous catalysis, in particular realistic catalytic systems with direct relevance to industrial applications. He stressed that catalysts are complex and disordered materials that need to be measured under operating conditions in order to understand the correlation between their functionality and surface chemistry. The following two talks by

Simon Mun and Hendrik Bluhm gave an overview of the APXPS facilities at beamlines 9.3.2 and 11.0.2 at the ALS. Both speakers also presented ongoing plans for future, next-generation APXPS endstations at both beam lines. John Hemminger's (UC Irvine) talk focussed on the application of APXPS to problems in atmospheric chemistry, in particular aerosol/vapor interfaces. In the next talk Gabor Somorjai (UC Berkeley) discussed the general need for in situ measurements in heterogeneous catalysis and discussed in particular two techniques that are complementary to APXPS, namely in situ scanning tunneling microscopy (STM) and in situ sum-frequency generation. The closing talk of the first day of the workshop was given jointly by Susumu Yamamoto and Lars-Åke Näslund (both SSRL) who presented recent data on the initial stages of water adsorption on metal and metal oxide surfaces, as well as the current status of the development of a dedicated APXPS endstation at SSRL.

The second day of the workshop was opened by Maya Kiskinova (Elettra, Trieste) who discussed recent results of APXPS experiments on the oxidation of ruthenium, and also the basic design considerations for a scanning APXPS instrument. Next Valerii Bukhtyiarov (Boreskov Institute of Catalysis, Novosibirsk) presented results of APXPS experiments on the epoxidation of ethylene over single and polycrystalline silver surfaces. He was followed by Dmitry Zemlyanov (Purdue University) who gave another example for the application of APXPS to the study of heterogeneous catalytic reactions, namely methane oxidation over palladium. Xingyi Deng (LBNL) then presented results from a combined in situ X-ray emission spectroscopy (performed at beamline 7.0.1 at the ALS) and APXPS study (beamline 11.0.2) of the oxidation and reduction of cobalt nanoparticles. This was followed by a talk by Andreas Thissen (SPECS GmbH, Berlin) who discussed design considerations for lab and synchrotron-based APXPS instruments, as well as the development of high-pressure (~20 bar) and high temperature cells for experiments in heterogeneous catalysis. Afterwards Simon Mun presented results from collaborative investigations with Francisco Aires (IRCE, Lyon), where a combination of STM, APXPS and X-ray diffraction methods was used to investigate the adsorption of carbon monoxide on a palladium-gold alloy. David Starr (Brookhaven National Lab) focussed in his talk on the adsorption and reaction of nitric oxide with 2…7 monolayer thick magnesium oxide films that were grown on silver substrates, where the reaction

depended strongly on the thickness of the magnesium oxide film. The workshop was concluded by a talk by Simon Bare (UOP, Chicago) who presented APXPS results on the oxidation and reduction of an industrial vanadium-molybdenum oxide catalyst, but in addition gave also a perspective on the role of APXPS for industrial catalysis applications.

The wide variety of applications of APXPS that were discussed during this workshop as well as the large number of participants from many international institutions demonstrated that during the last few years a robust and vibrant APXPS community has grown. A number of synchrotrons are now planning new APXPS facilities to satisfy the increasing demand for user time at APXPS endstations. The participants of the workshop agreed that there is a need for frequent meetings of the APXPS community, and it was therefore suggested that this workshop will be held annually, with the location alternating between the US (Berkeley) and Europe (Bessy, Berlin and Elettra, Trieste).

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