UV Photoelectron Spectroscopy at Near Ambient Pressures : An Unique Tool to Explore Electronic Structure under *in-situ* conditions

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Abstract

Near-ambient pressure photoelectron spectroscopy (NAPPES) is becoming increasingly popular to explore the surface science and catalysis aspects at near ambient pressure (around 1 mbar and higher) and high temperature conditions. NAPPES works fine with x-ray photons, or rather high kinetic energy (KE) electrons, mainly due to relatively low inelastic scattering and hence good S/N can be maintained. However, when the KE of photoelectrons are <100 eV, there are serious problems in observing the spectra with decent S/N ratio under NAPPES conditions. In the recently installed laboratory-based NAPPES system at NCL, Pune,[1] we are able to observe the ultraviolet PES (NAP-UPS) with He-I and He-II excitation sources under near ambient conditions. Figure 1 shows the NAP-UPS spectrum obtained on Ag-surfaces at room temperature and different partial pressure of N_2. Indeed well-defined electronic and vibrational states of molecular N_2 was also observed between 11 and 15 eV. As a test case we explored the (a) oxidation of polycrystalline copper surfaces under molecular O_2 at different partial pressures and temperatures,[2] and (b) reduction of $Ce_{0.95}Zr_{0.05}O_2$ in H_2.[3] Changes observed in the valence band spectra were recorded with AlKα, and NAP-UPS with He-I for systematic changes in oxidation of metallic Cu to CuO through Cu_2O. Similar analysis was made for $Ce_{0.95}Zr_{0.05}O_2$ surfaces. The most important point is the observation of UPS under high pressure conditions, which demonstrate the possibility of exploring low KE electrons under NAPPES conditions. Important features of APPES unit available at NCL will be presented in detail (Fig. 2).

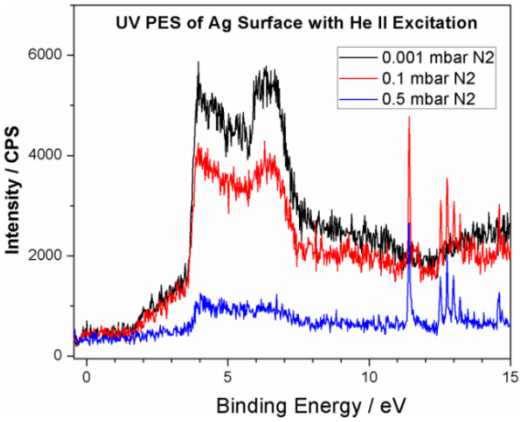

Figure 1: Valence band spectra recorded on Ag foil with He II source at different partial pressure of N_2.

Figure 2: Digital photograph of the custom-built NAPPES system available at NCL, Pune.

References:

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2. K. Roy C. S. Gopinath, *Anal. Chem.* **86**, 3683 (2014).
3. R. Jain, A. Dubey, M.K. Ghosalya, C. S. Gopinath, *Catal. Sci. Techno.* **6**, 1746 (2016).