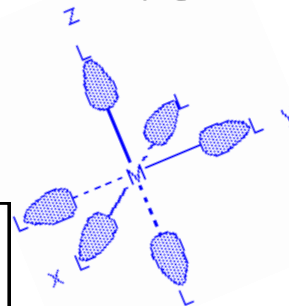


New Developments for the Analysis of XPS

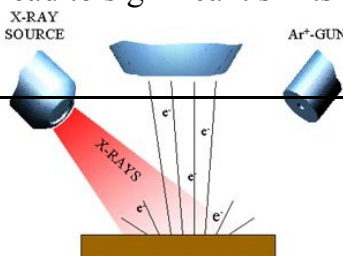


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X-Ray photoelectron spectroscopy, XPS, has a great potential for providing information about the electronic structure of matter; in particular, information that goes far beyond determining elemental composition. The properties of the spectra that one wishes to

understand include: the energy shifts of peaks between an atom in different environments; the energies and intensities of multiplet and satellite peaks and the broadening of peaks. Our recent rigorous theoretical studies of the chemical and physical origins of these features provide understandings that are different from many commonly held beliefs. Our goal is to relate features of XPS spectra to the chemistry of the material. We show that the vibrational broadening of XPS peaks provides chemical information. We also analyze the interactions in ionic metal oxides in terms of the covalent mixing of the metal and ligand orbitals and we show how this is related to the XPS satellites. Finally, we show that the hybridization of orbitals to facilitate chemical bonding may lead to significant shifts of the XPS binding energies.



**Physics and Astronomy
& NCMN**
2011 Fall Colloquium

29 September 2011

Lecture: 4:00 pm, 110 JH

Refreshments: 3:30 pm, 1st Floor Vending Area