# LECTURE

VISITING PROFESSOR PROGRAMME

## *Professor Paul Bagus*

University of North Texas, USA

and Connie J. Nelin
Consultant, Austin, TX, USA

will deliver a lecture titled:

## *Extracting Chemistry From the Analysis of Core-Level Spectra*

***DATE:*** Thursday, 30 May 2019 | 11.00
***VENUE:*** CNBCh, seminar room 0.38

ABSTRACT:

X-Ray Photo-electron Spectroscopy, XPS, is widely used to obtain information about both the composition and the chemical bonding of materials. The interpretation of the XPS in terms of chemical interactions is very commonly focussed on the shifts of core-level binding energies, BEs, to infer the chemical state of the material. In particular, a shift to higher BE is taken as indicating that the ionized atom is more positively charged, and the reverse is taken for shifts to lower BEs. However, there are other reasons for shifts in BEs besides charging; these include changes in hybridization and changes in bond distance. Furthermore, there are other features of the XPS besides BE shifts from which chemical properties of the material can be inferred. These include the number, width, and relative intensity of the main and satellite peaks of the often complex XPS spectra. The physical and chemical origins of these features allow them to be related, especially with guidance from theory, to the electronic structure of the material. An important mechanism is the angular momentum coupling of the open shell electrons which often leads to unresolved features and broad observed peaks.

Activity at Home University: The principle scientific interest of prof. Paul Bagus is to develop and apply theory and computation for the interpretation of core-level spectroscopies including XPS, XAS, and XMCD. These spectroscopies are routinely used non-destructive probes of material composition and properties. The aid of theory is needed for proper interpretation of these spectroscopies in terms of materials properties. Bagus' work on chemisorption has involved the use of cluster models to represent the surface electronic structure and, in particular, to describe the chemical interaction of adsorbed atoms and molecules with the surface. A special advantage of the cluster model is that it naturally allows chemical concepts to be used to interpret surface chemical bonding and surface reaction processes. His work related to surface electronic structure has addressed how this structure leads to observable properties. These have included work function changes, surface and nano-particle core-level binding energy shifts, and the nature of the chemisorption bond between adsorbates and substrates. For this latter research, he and his collaborators have developed a theoretical methodology that has allowed them to decompose different contributions to the chemisorption bond.

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