# LECTURE

VISITING PROFESSOR PROGRAMME

# Professor Paul Bagus

University:

University of North Texas, USA

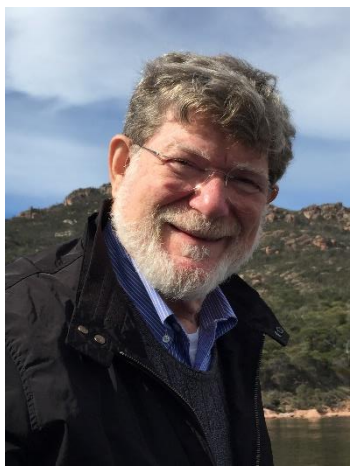
will deliver a lecture titled:

## Multiplets: A Tutorial

**DATE:** Monday, 3 June 2019 | 11.00
**VENUE:** CNBCh, seminar room 0.38

ABSTRACT:

A knowledge of multiplets is essential to understanding and interpreting all electronic spectra. This is true for both core and valence level spectroscopies. Multiplets have their origin in the angular momentum coupling of open shell electrons. They are the basis of selection rules and provide important information about the complexity of spectra including energy separations and relative intensities. A difficulty is that the fundamental theory of angular momentum coupling is based on a complex mathematical formalism. The objective of this tutorial is to show that there are simple rules that provide important information about the properties of multiplets and provide guidance for how the multiplet structure will be reflected in the electronic spectra.



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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