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:

Theoretical Analysis and Understanding of Chemisorption

DATE: Tuesday, 28 May 2019 | 9.30
VENUE: CNBCh, seminar room 0.37

ABSTRACT:
The objective of this presentation is to show how chemisorption bonds can be analysed to identify the chemical and physical mechanisms responsible for the interaction and to show the consequences of the interaction for observed properties. An important result of this understanding is that it makes possible the correct interpretation of the relationship of observed properties to the nature of the surface chemical bond. The authors and their colleagues have pioneered in the development and application of theoretical methods that make it possible to identify the character of chemical interactions in terms of the concepts of molecular orbital theory. These methods will be applied to describe the bonding of common probe molecules, CO, CN, and NO, to different surfaces, including metals and insulators where the focus will be on the chemical content of the analysis rather than on the computational methods. The analysis will include interpretation of vibrational and photoemission spectroscopies and it will be shown how these spectra reflect the adsorbate-substrate interaction.

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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