NEW TECHNOLOGIES
RESEARCH CENTRE
UNIVERSITY
OF WEST BOHEMIA

INVITATION

New Technologies – Research Centre

Is proud to invite you to the lecture

Treating strong correlation effects in materials science: a DMFT perspective

by

prof. Dr. Igor Di Marco

Materials Theory Division, Department of Physics and Astronomy, Uppsala University, Sweden

Department of Physics, Pohang Institute of Science and Technology (POSTECH), Gyeongbuk 790-784, Pohang, South Korea

In the last decade the combination of dynamical mean-field theory (DMFT) and density functional theory (DFT) has emerged as a very powerful approach to investigate the electronic structure of strongly correlated materials. This technique, labeled as the DFT+DMFT scheme, will be the main topic of the present talk. I will first introduce the basic concepts of strong correlations in solids and provide a brief description of DFT, DMFT and DFT+DMFT. After this introduction, I will illustrate how strong electronic correlations affect the electronic structure of certain classes of materials, including the late transition metals and their oxides. I will then focus on the whole series of the elemental Lanthanides, which are very difficult to describe in standard DFT. I will show that the DFT+DMFT scheme is capable of describing electronic and magnetic properties with a great accuracy and can be very helpful for engineering new materials containing Lanthanides, as e.g. novel permanent magnets. I will finally present my latest work, on modeling X-ray absorption spectroscopy (XAS) within DFT+DMFT.

Date: **9 August 2018**

Time: **14:00**

Venue: **Building C1 Vědeckotechnický park, room TC211, Teslova 5B, Pilsen**

This lecture was supported by the project CEDAMNF, reg. no. CZ.02.1.01/0.0/0.0/15_003/0000358, co-funded by the European Regional Development Fund (ERDF).

EUROPEAN UNION
European Structural and Investment Funds
Operational Programme Research, Development and Education

MINISTRY OF EDUCATION, YOUTH AND SPORTS