

## SEMINARIUM RENTGENOWSKIE

Dnia 17.04.2012 r. o godz. 10.30, w sali D Instytutu Fizyki PAN, odbędzie się seminarium, na którym dr Iraida N. Demchenko z Instytutu Fizyki PAN wygłosi referat p.t.:

### *"Investigation of electronic structure of materials by x-ray spectroscopies - part 2"*

Abstract:

A detailed interpretation of x-ray absorption near edge structure at the  $K$  and  $L_3$  edges of oxygen and cadmium in CdO film within the *ab initio* full multiple-scattering formalism (FEFF8 code) will be present. Based on the real-space multiple scattering approach it makes possible to interpret the experimental spectra in terms of local geometrical and electronic structures. Calculated near-edge structure for cation and anion x-ray absorption edges represents a good coincidence with the experimental one. Not purely ionic bonding in CdO is identified. Calculated PDOS describes well all features corresponding to unoccupied states of investigated films and allows concluding that the orbital character of the lowest energy of the CB is mostly of Cd  $5s$ -O  $2p$   $\sigma^*$ . It will be shown that the resonant inelastic X-ray scattering (RIXS) CdO data set is showing a progressively varying partial  $k$  mixing of initial and final states near the threshold and thus a varying incoherent line shape. Overlapping of XAS spectrum with RIXS ones makes possible to estimate both direct  $\sim 2.4$  eV and indirect  $\sim 0.9$  eV bandgap values. The obtained results are consistent with the theoretical/experimental ones presented in the literature and our own optical absorption results.

Dr Ryszard Sobierajski