



G-RISC
German-Russian
Interdisciplinary
Science Center



Санкт-Петербургский
государственный
университет

Public Lectures (Part I)

Nanoscale atomic and electronic structure of materials: X-ray spectroscopy and theoretical insight

Professor Dr. Alexander V. Soldatov

Research center for Nanoscale Structure of Matter
Southern Federal University, Russia

Tuesday, 22. June 2010, 10:00 – 13:00
Takustr. 3, 14195 Berlin, Seminar Room 12.12

Lecture I (10:00 – 10:45)

Introduction: Atomic structure, electronic structure and physical properties

Interplay between local atomic structure and electronic structure of materials. Basic concepts of electronic structure and its main parameters. Connection of electronic structure with observed physical properties of the materials: electron conductivity, magnetic properties, optical properties.

Lecture II (11:00 – 11:45)

X-ray Spectroscopic techniques

XAFS spectroscopy (XANES, NEXAFS, EXAFS) comparison to TEM based EELS spectroscopy (ELNES). XES spectroscopy. XMCD spectroscopy.

Lecture III (12:00 – 12:45)

Theoretical methods for electronic structure and x-ray spectroscopy data analysis

DFT formalism. Band structure theory. KKR formalism. APW methods. Multiple scattering in real space. Finite differences method in real space. Muffin-tin approximation for the potential- “pro and contra”. A review of existing software codes.



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Public Lectures (Part II)

Nanoscale atomic and electronic structure of materials: X-ray spectroscopy and theoretical insight

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Friday, 25. June 2010, 14:00 – 17:30
Takustr. 3, 14195 Berlin, Seminar Room 12.12

Lecture IV (14:00 – 14:45)

Nanoscale local atomic structure of the materials on the basis of advanced theoretical analysis of x-ray spectroscopic experiments

FitIt approach for the extraction of local atomic structure parameters from XANES (NEXAFS, EELS) data.. *CD Disk with the FitIt 2.0 software and tutorials will be available for the participants of the course*

Lecture V (15:00 – 15:45)

Case studies

nanoclusters, metalloproteins, intermediates in chemical reactions, catalysts.

**This lecture is followed by a coffee break and a related Special Seminar in the same
room (16:15-17:30):**

Prof. Dr. Nobuhiro Kosugi

UVSOR. IMS, Myodaiji, Okazaki 444-8585, Japan

Inner-Shell Spectra of Weakly-Bound Systems