Computation Physics in the Institute for Metal Physics

1973-2013

Computers:

1974 -- 1987	**ES-1022**
1978--1995	**BESM-6**
1987--1996	**ES-1055**
Since 1990	**PCs**
Since 2007	**GRID Cluster**

Organization

1975-2013

1975 -- 1979	**Computer Laboratory, Institute of Metal Physics**
1979 – 1990	**Computer Department, OKTB IMP**
1982 – 1987	**Computational Physics Laboratory, IMP**
Since 1987	**Computational Physics Department, IMP**

Computational Methods and Computer Codes:

1974 - 1978 Augmented Plane Wave method (APW, RAPW)
(V. Antonov, Vl. Antonov, A. Timoshevskii)

1974 - 1978 X-alpha Scattered Waves method
(Y. Kucherenko, L. Sheludchenko, A. Yaresko)

1982 – 1984 Linear Augmented Plane Wave method (LAPW)
(N. Plotnikov)

1983 – 1985 Relativistic Dirac LMTO method (RLMTO)
(A. Krasovskii)

1984 – 1988	Linear Augmented Plane Wave method (LAPW) » (E. Krasovskii, M. Miller)
1984-1988	Relativistic First Principle Pseudopotential Method (V. Milman)
1985 – 1990	Linear Muffin-Tin Orbial method (LMTO) (A. Baglyuk, A. Perlov, A. Yaresko)
1995 – 2013	Relativistic Spin-Polarized LMTO method (A. Yaresko, A. Pelov)

Soft x-ray emission spectroscopy

- A new method for the calculation of the intensity of soft x-ray emission (SXE) spectra on the basis of Dirac equation was derived.
- 1973 – 1976 The electronic structure and SXE spectra of 4*d* transition metals. (V. Antonov)
- 1976 – 1979 The electronic structure and SXE spectra of 5*d* transition metals. (Vl. Antonov)
- 1979 – 1982 The electronic structure and SXE spectra of transition metal compounds. (N. Plotnikov)

V.V. Nemoshkalenko, V.N. Antonov, *Computational Methods: Band Theory of Metals. - Kiev, Naukova Dumka, 1985, 408 p. (in Russian).*

V.V. Nemoshkalenko, V.N. Antonov, *Computational Methods in Solid State Physics.- Gordon and Breach Publishers, 1998,314 p.*

Electron spectroscopy

- Methods for the calculation of the intensity distribution in the electron emission spectra taking into account transition probabilities from different electron states were derived
- 1973 – 1979 X-ray photoemission spectra of transition metals, alloys and compounds (Yu. Kucherenko, L. Sheludchenko)
- 1980 – 1994 Auger electron spectra of metals and compounds (Yu. Kucherenko)
- 1995 – 2000 Photoelectron diffraction on the crystalline lattice (P. Rennert, Yu. Kucherenko)
- 1998 – 2012 Resonant photoemission spectra of rare-earth metals and compounds (Yu. Kucherenko)

Electronic structure in non-perfect crystals

- 1973 – 1976 Disordered alloys of transition metals by means of Coherent potential approximation

  (Yu.Kucherenko, L.Sheludchenko)

  1976 – 1986 Point defects in metals and compounds by means of cluster X-alpha scattered waves (Yu.Kucherenko, L.Sheludchenko)

  1988 – 1993 Point defects in metals by means of LMTO-Green-function method

  (A. Perlov, Yu. Kucherenko, V. Antonov)

V.V. Nemoshkalenko, Yu. N. Kucherenko, Computational methods: Electronic states in non-perfect crystals *- Kiev, Naukova Dumka, 1985, 295 p. (in Russian).*

Electron-phonon interaction

A new method for the calculation of the electron-phonon interaction (EPI) on the basis of Dirac equation was derived

(W. John, V. Antonov, 1980).

1980 – 1981 *The electron-phonon interaction in 5d transition metals.*
(W. John and V. Antonov)

1982 – 1983 *Nuclear Spin-Lattice Relaxation Time in 5d metals.*
(W. John and V. Antonov)

1987 *The Gyromagnetic (g-) factor of conduction electrons .*
(C. Schober and V. Antonov)

Fermi surface and electron-phonon interaction

Fermi surface*:* Fermi surface topology, extremal diameters, extremal momenta, the orientation dependence of extremal cross-section areas and cyclotron masses.

These results have been used to explain the de Haas-van Alphen effect, Sondheimer effect, magneto-acoustic and radio-frequency size effects, Doppler-shifted cyclotron resonance and anomalous skin-effects in 5d metals and transition metal silicides and diborides.

- **Electron-phonon interaction:** *Elliashberg function, point-contact spectral function, the constant of electron-phonon interaction, the transport spectral function, temperature dependence of phonon resistivity*

Fermi surface and electron-phonon interaction

1980 – 1988 *The Fermi surface properties and electron-phonon interaction in 5d metals and compounds.*

(A. Zhalko-Titarenko)

1982 – 1985 *The Fermi surface properties of transition metal silicides.*

(B. Yavorsky)

2005 – 2013 *The Fermi surface and EPI from "first principles" in hcp transition metals and transition metal diborides.*

(S. Sichkar)

Martensitic phase transformations

- First principles calculations of total energies and atomic forces are used to evaluate the stability, transformation paths, and the role of alloying and defects in materials undergoing structural phase transformations.
- **We discover that martensitic phase transformation in TiNi and PdNi is accompanied by a strong reconstruction of the Fermi surface (Lifshitz 2 1/2 phase transition).**

(M. Miller: 1988 – 1991)

- Our research in the Martensitic Phase Transformation phenomena have been recognized by the G.V. Kurdyumov Award of Ukrainian National Academy of Sciences in 1999

(**V. N. Antonov, V.V. Nemoshkalenko, and Yu.N. Koval**).

Lattice dynamics

- **Lattice dynamics from "first principles"**: *Norm conserved "first principle" fully relativistic pseudopotential method was derived*

- **Lattice properties:** *elastic constants and their pressure derivatives, P-V equation of state, lattice specific heat, the microscopic Gruneisen parameter, phonon dispersion curves and phonon density of states.*

- **1984 – 1989** *Lattice properties of transition metals including 5d metals were investigated in details.*

  (V. Milman)

High-Tc superconductivity

1. Electronic structure and Fermi surface of $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_7$ superconductors
2. Electronic structure and Fermi surface of Bi-Sr-Ca-Cu-O superconductor

(**V.V. Nemoshkalenko, V. Antonov, V.G. Bar'yakhtar, A. Baglyuk,** ***A. Zhalko-Titarenko, 1988 – 1993***)

3. Optical conductivity of superconducting Rb2Fe4Se5 single crystals
4. The electronic structure and physical properties of $SrPd_2Ge_2$, LiFeAs, BaKFeAs and other superconductors

(**A. Yaresko*, 2009 – 2013***).

Optical properties

- **Optical properties**: *dielectric tensor, optical reflectivity, optical absorption, energy-loss spectra, electron-photon emission, photo-electron spectra, LEED spectra, etr.*
- *A fully relativistic treatment of the optical properties based on Dirac equation has been developed (*A. Baglyuk, A. Perlov, 1989*).*
- *Optical properties of **5d** transition metals (*A. Baglyuk, A. Perlov, V. Antonov, V.V. Nemoshkalenko, 1990-1992*).*
- *Optical properties of **3d** and **4d** transition metals and their compounds (*E. Krasovskii, V.V. Nemoshkalenko,1989-1993*).*
- *Theoretical study of optical and ultraviolet photoemission spectra of transition metal oxides, diborides, hydrides, topological insulators, etr. (*E. Krasovskii 1993-2013*).*
- *Electron-photon emission in solids (Y. Kulupin, E. Krasovskii, V.V. Nemoshkalenko, V. Shatalov, 1986-1989).*

Magneto-optical properties

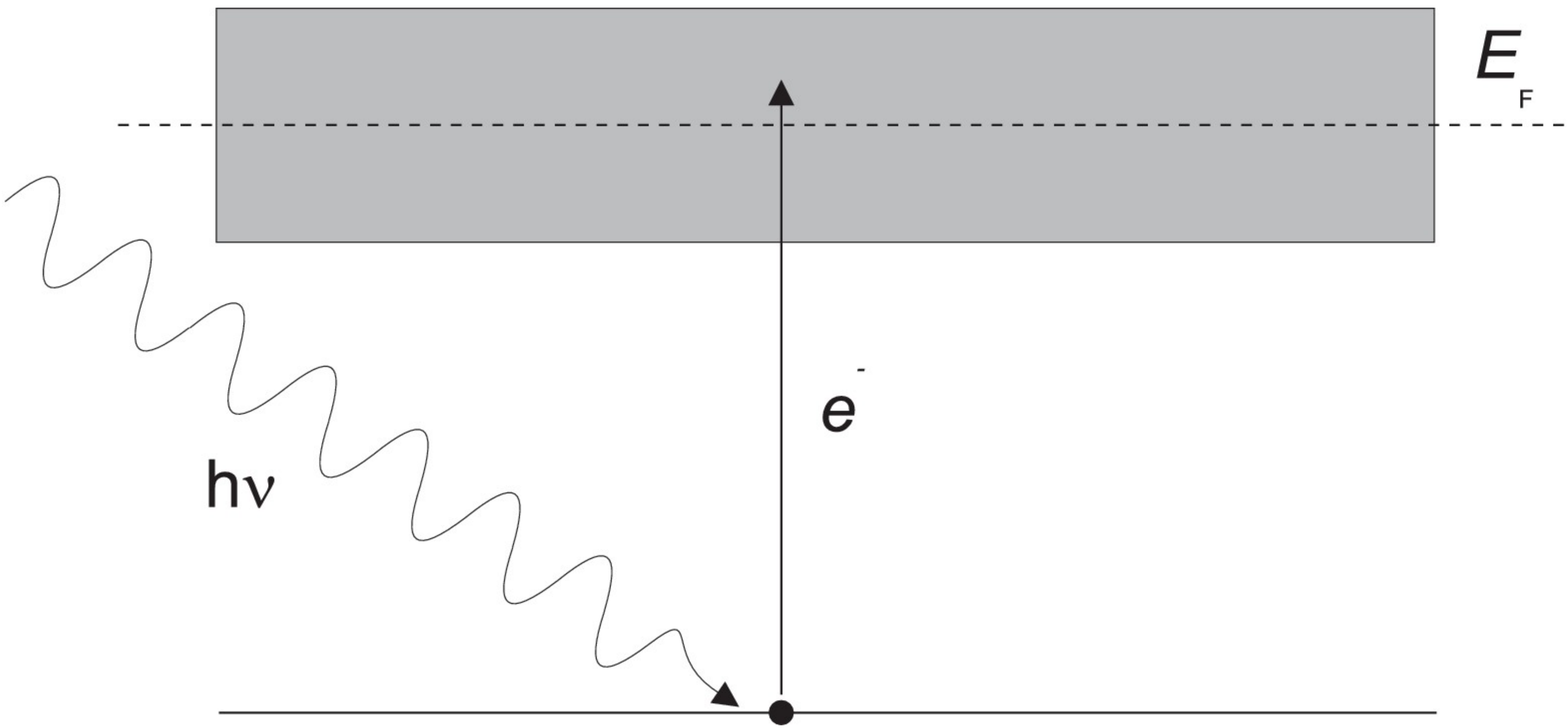
- A fully relativistic treatment of the magneto-optical properties based on Dirac equation has been developed.
- The method was applied to *5d* transition metals and to *5f* early actinides. The anisotropy of the optical properties of some transition metal silicides has been calculated.
- In 90's we deal with magneto-optical (MO) properties of solids. We derived fully relativistic spin-polarized LMTO method and applied to: transition and noble metals, ternary Heusler type alloys, magnetic transition metal platinum alloys, chromium spinel chalcogenides, some uranium compounds and transition metal multilayers.
- We predict several materials that could be promising for MO recording. We also propose a set of guidelines for the future predictions of materials having suitable MO properties.

- **V.N. Antonov, B.N. Harmon, and A.N. Yaresko**, *Electronic Structure and Magneto-Optical Properties of Solids.* - Kluwer Academic Publisher, 2004, 518 p.

Strongly correlated electron systems

- Physical properties arise from the correlations among electrons: metal-insulator transitions, valence fluctuations, heavy fermion behavior, superconductivity, charge and orbital ordring, etr.
- The electronic structure and physical properties: *4f* charge-fluctuating mixed-valence compounds (*TmSe, SmS*, SmB_6, $YbInCu_4$, Yb_4As_3, Sm_3S_4 and Eu_3S_4); charge-ordering, metal-insulator transition metal oxides (Fe_3O_4, Fe_2OBO_3, NaV_2O_5, $MgVO_3$); heavy fermion compounds (*YbIr2Si2*,*YbPtBi*, UPt_3, URu_2Si_2, UPd_2A_3, and UBe_{13}); compound with a giant magnetocaloric effect $Gd_5(Si_2Ge_2)$ and so on.
- Topics of particular current interest include the interplay between charge, orbital and spin degrees of freedom in these systems.
- To treat the electron-electron correlation we used the rotationally invariant LSDA+U method. We used the 'relativistic' generalization of the LSDA+U method derived by (A. Yaresko, 2003) which takes into account spin orbit coupling.
- (**A. Yaresko, Yu. Kucherenko, V. Antonov, 1995 – 2013**)

X-ray magnetic circular dichroism



X-ray magnetic circular dichroism (XMCD)

- This is a new technique made possible by the advent of highly intense synchrotron facilities. The difference in absorption between left and right circularly polarized X-rays at a core edge gives information about the size of the local magnetic spin and orbital moments which arise from spin-orbit coupling.
- The results are element and angular momentum specific, so one may learn a great deal about microscopic magnetic interactions.
- We are the leaders in the world in calculating the expected theoretical profiles and are working with different experimental groups in developing the method for general utility.
- Our most recent effort was a complete evaluation of XMCD edges for magnetic transition metal platinum alloys which are used in magnetic recording thin films.

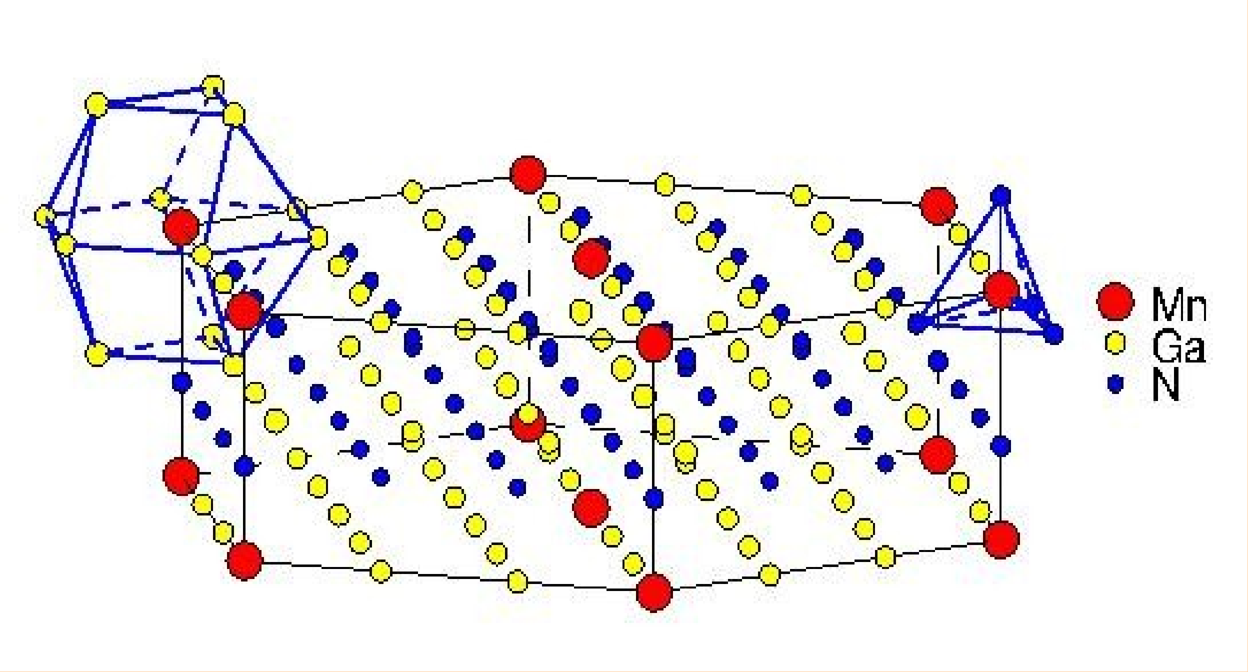
A. Perlov, A. Yaresko, L. Bekenov, D. Kukusta, V. Antonov, 1999-2013

X-ray magnetic dichroism in the III−V diluted magnetic semiconductors

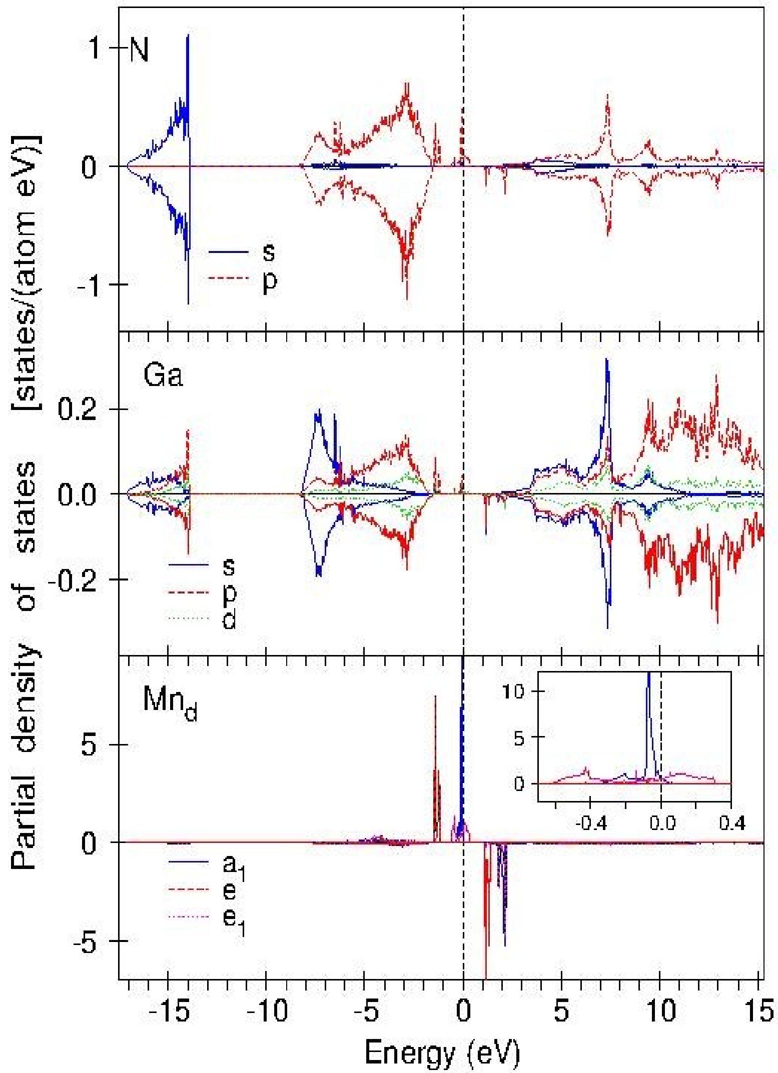
V. Antonov, A. Yaresko, and O. Jepsen

- **Diluted magnetic semiconductors (DMSs) are semiconductors alloyed with magnetic elements. The physical properties of these materials can be tuned by both charge and spin, thus, they have great potential of being used in a wide variety of spintronic applications, such as magneto-optical, magneto-electrical, and magneto-transport devices. devices.**
- **In this respect Mn-doped III-V semiconductors are among the most frequently studied. Mn doped DMSs are most suitable for spintronic applications since the Mn ion possess the largest magnetic moment compared to other 3d transitional metals and it also creates a fully polarized stable state due to its half-filled 3d bands.**

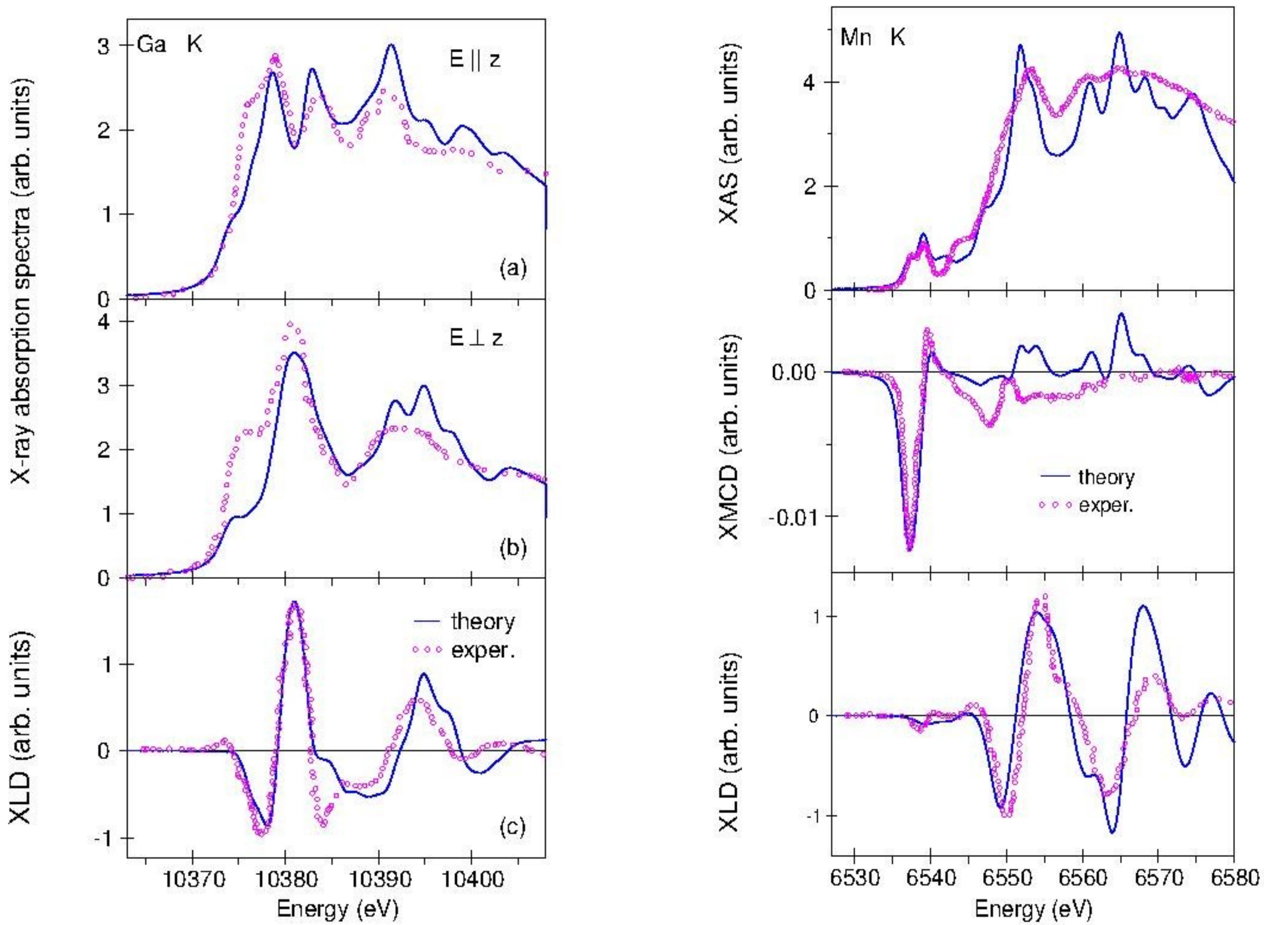
Crystal strcture of the $(Ga_{1-x}Mn_x)N$ (x=0.06)



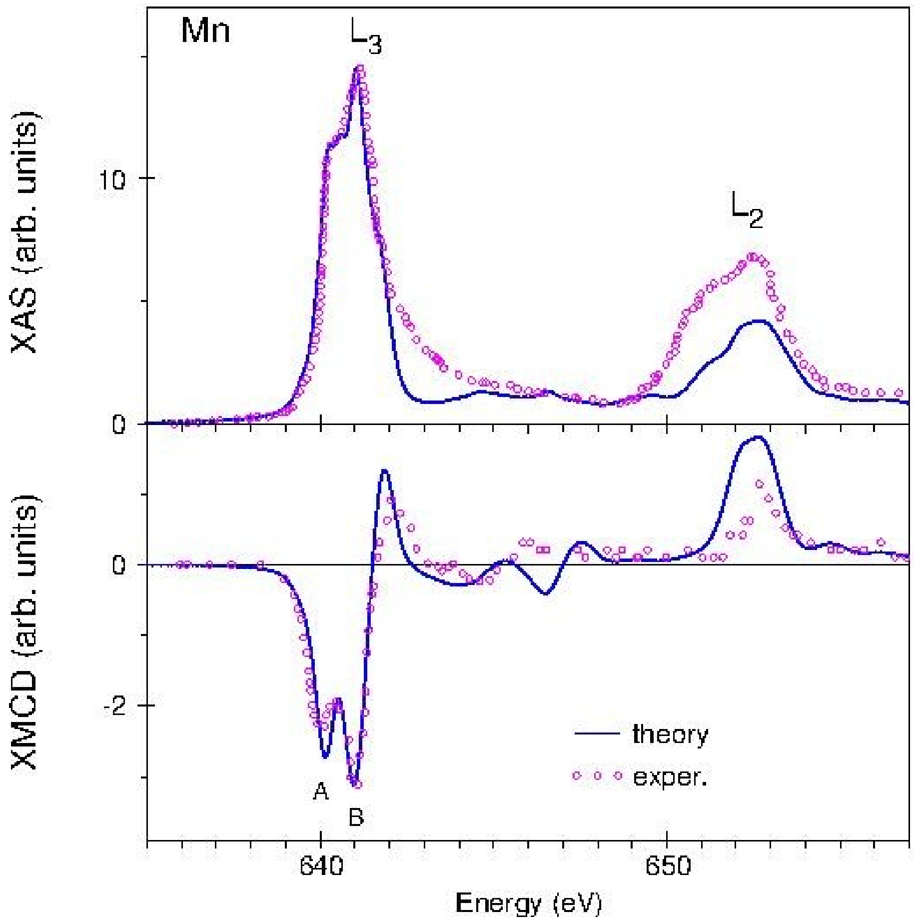
Partial densities of states



Ga K- and Mn K- XAS and XMCD spectra



Mn $L_{2,3}$ XAS and XMCD spectra



Publications:

560 publications including 15 review papers and 4 monographs

• Nature		3
• Phys. Rev. Letters,	Europhys. Letters	31
• Phys. Rev. B		121
• J. Phys.: Condensed Matter		32

• Low Temp. Physics		23
• Z. Phys. B,	Phys. Status Solodi B	31
• J. Electron Spectr.	J. Alloy and Compounds	23
• J. Appl. Physics,	Thin Solid Films	31
• Physica B	Solid State Commun.	29
• JMMM,	J. Phys. Chem. Solids	12