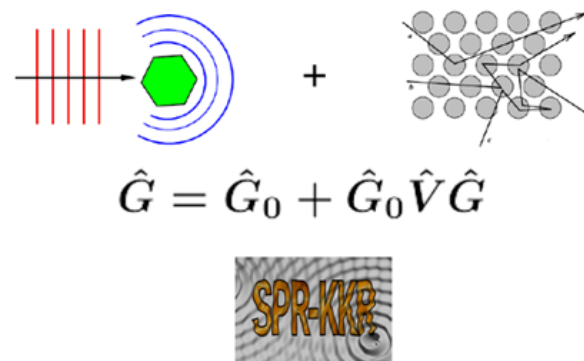
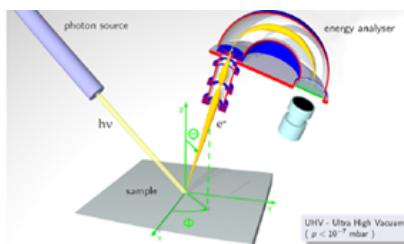


Computational and experimental design of advanced materials with new functionalities

Ján Minár

Department of Advanced Materials

University of West Bohemia, New Technologies-Research Center, Pilsen, Czech Republic



Macroscopical point of view

Magnetite (Fe_3O_4)



SiO_2

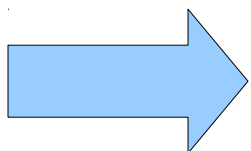


Macroscopical point of view

Magnetite (Fe_3O_4)



SiO_2

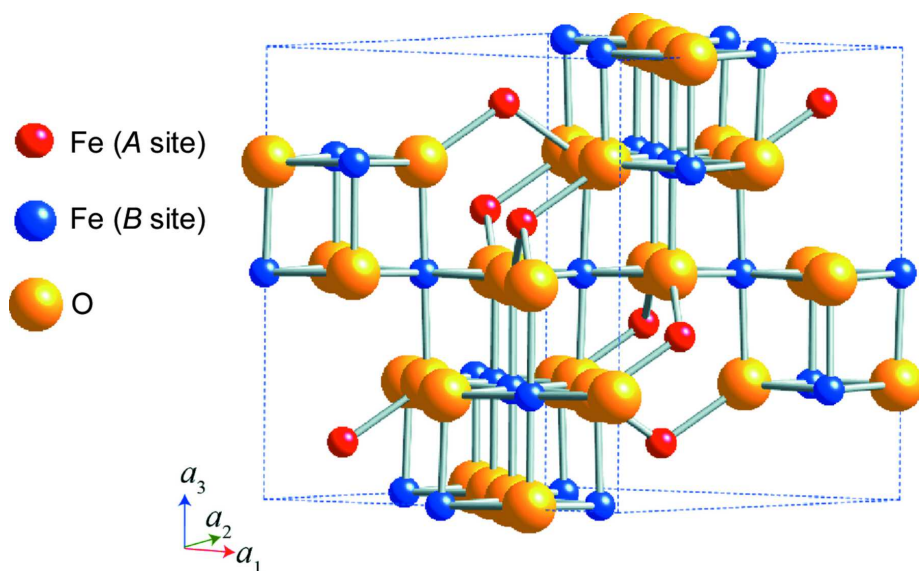


Technology

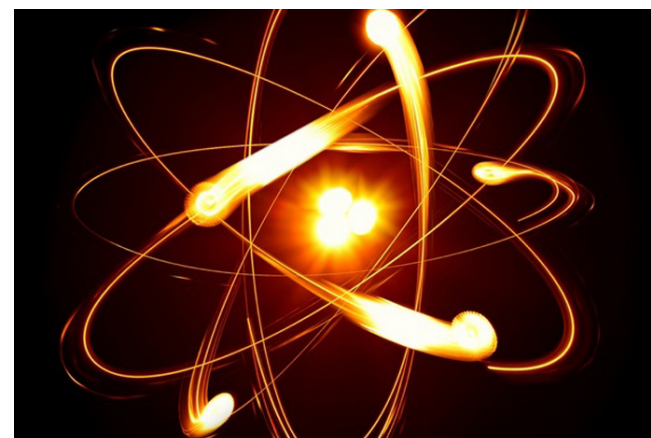


Microscopical point of view

Example: Magnetite (Fe_3O_4)



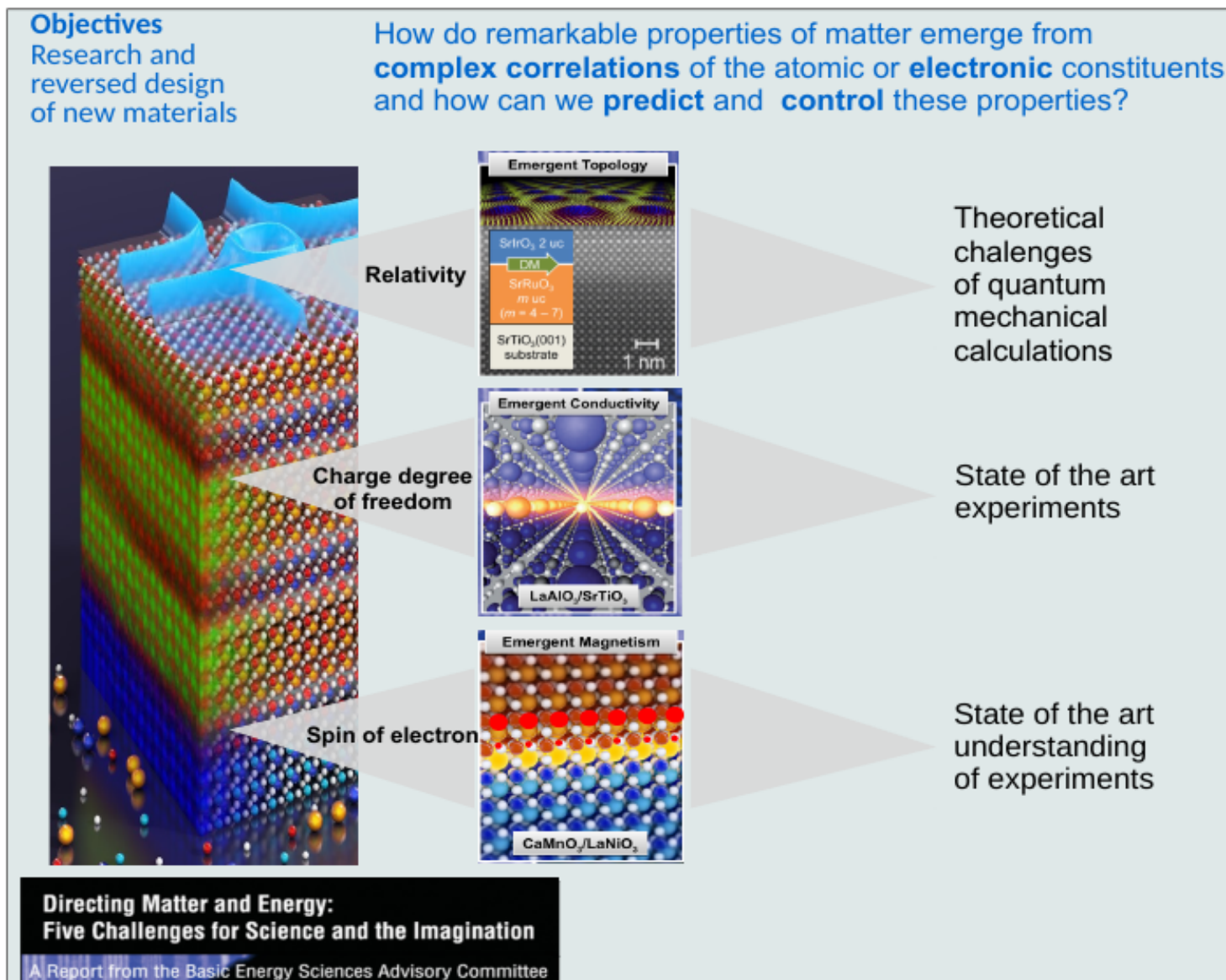
**Lattice
of positively charged ions**



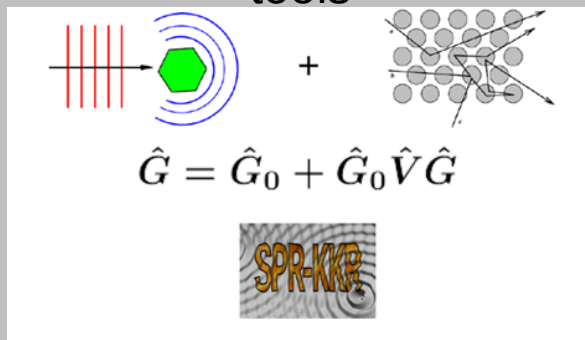
Electrons (-)

Charge, Spin, Mass,
Coulomb interaction

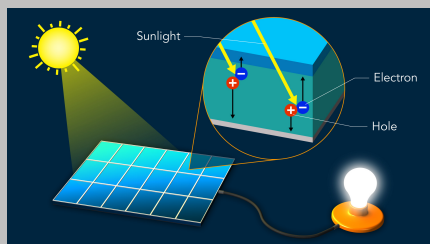
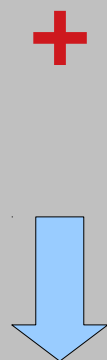
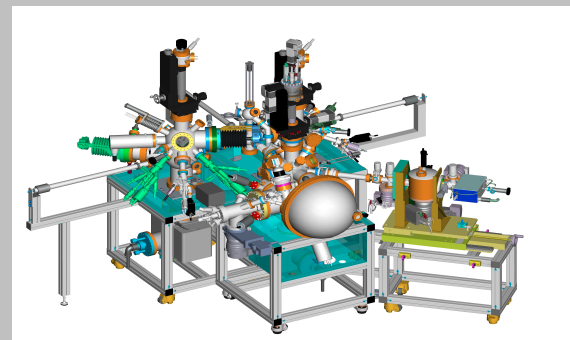
Physical foundations of material properties with special emphasis on electronic structure, magnetism and spectroscopy.



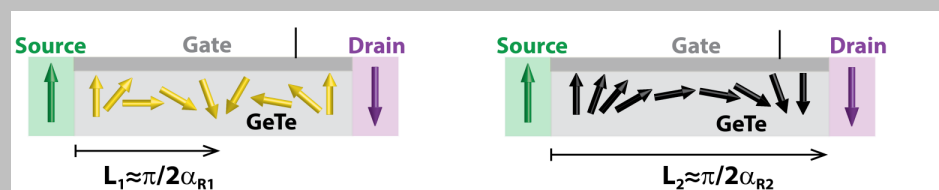
Development of theoretical tools



Understanding and developing of Experiments and spectroscopy

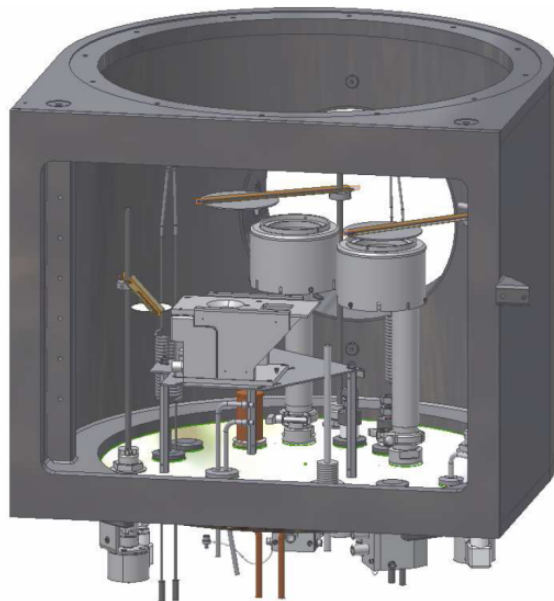


Si-based solar cells
 Perovskite based solar cells
 Transparent conducting oxides
 Phosphor-converted LED

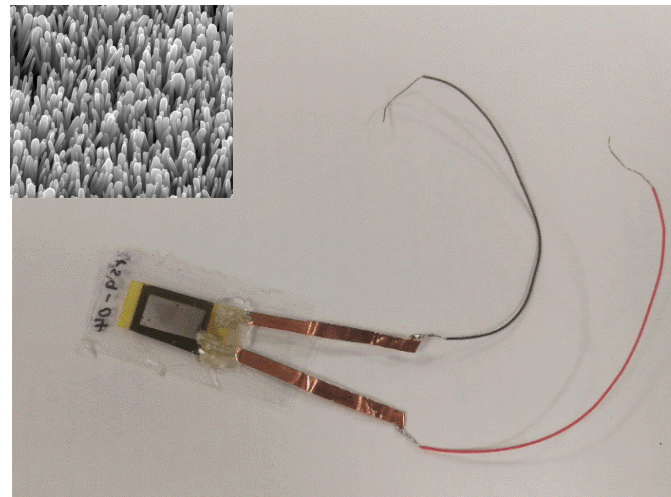
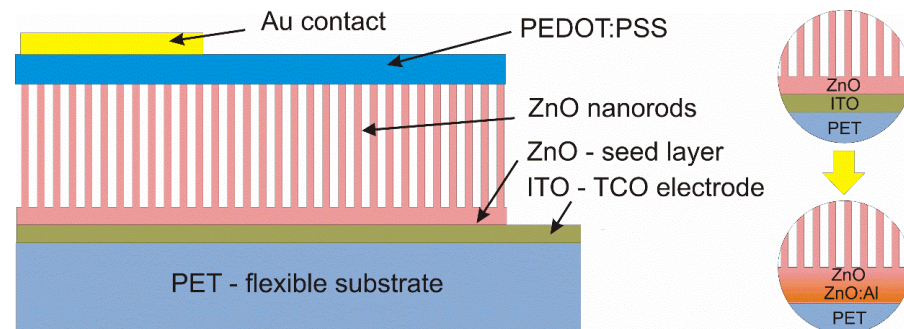


Magnetically doped semiconductors
 Topological materials and their surfaces
 Magnetic nano-structures

Magnetron sputtering and electron beam evaporation



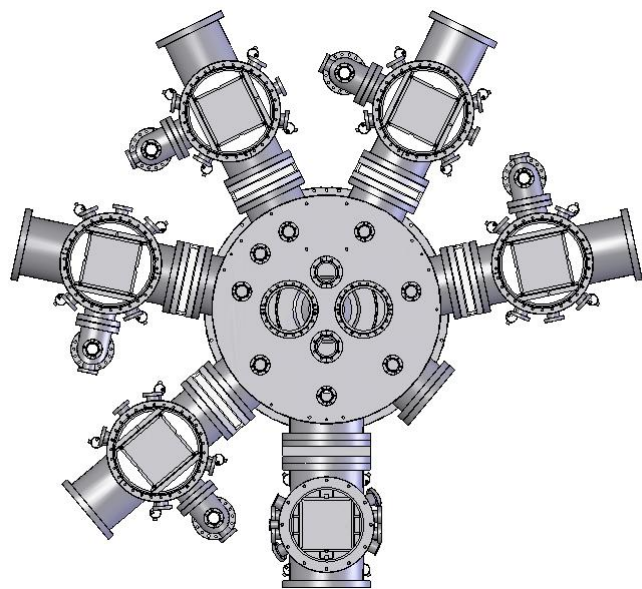
ZnO nanorod-based piezogenerator



Main Objectives

- Optimization of structure and electrical properties of ZnO seed layer
- Replacement of usually used indium doped SnO by aluminium doped ZnO films

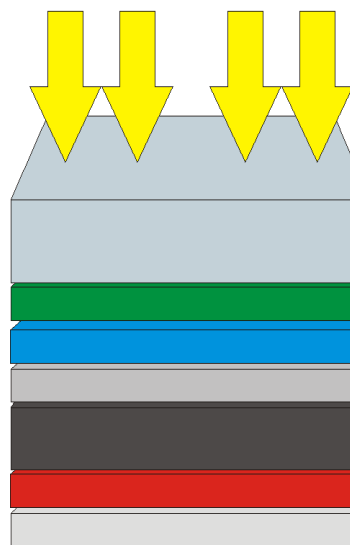
Elettrorava ClusterTool PECVD system



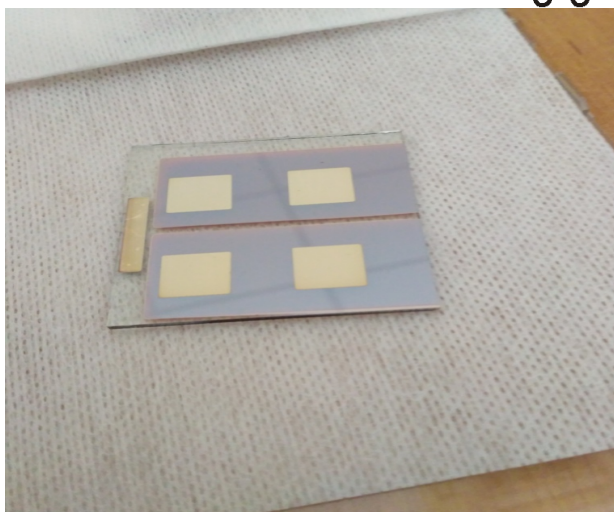
P. Calta et al., Vacuum 153 (2018) 154-161

Prototype of complete solar cell

Sun light



- Glass substrate
- ITO or FTO (~100-200nm)
- p-a-Si:H/p-a-SiC (~15nm)
- i-a-SiC:H (~5nm)
- i-a-Si (~300nm)
- n-a-Si:H (~20nm)
- Ag grids

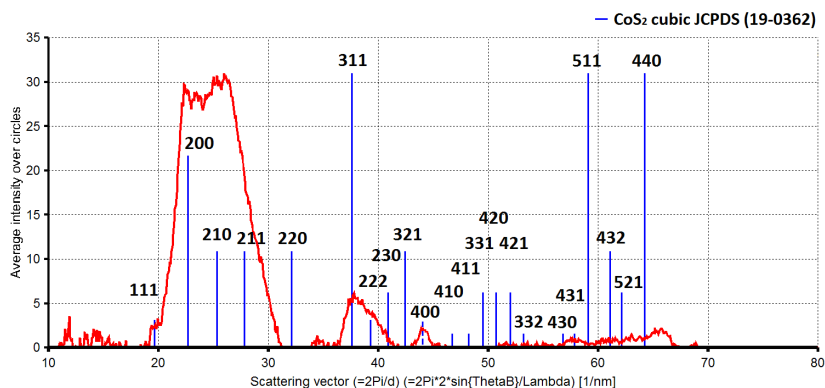


P. Calta et al.,
In preparation

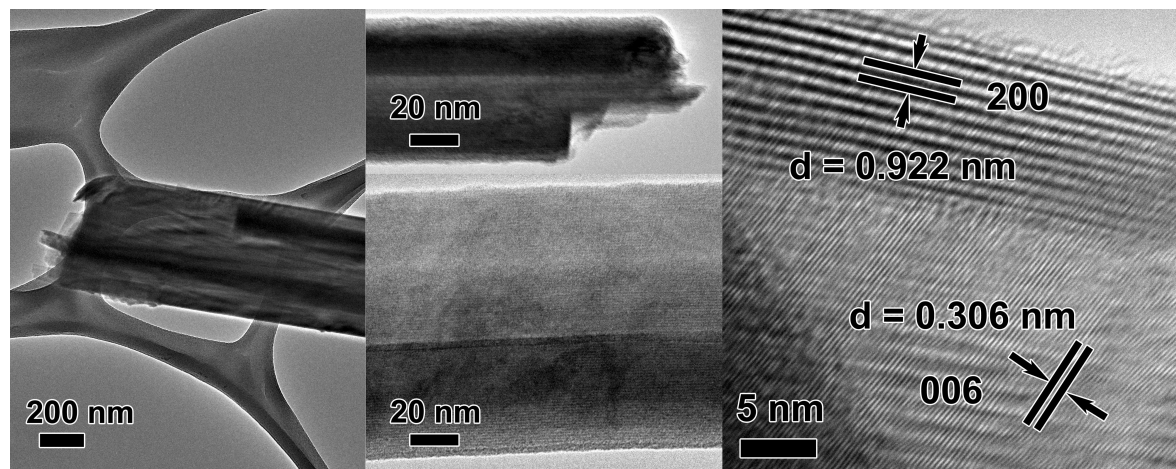
Electron microscopy and X-ray diffraction



TEM JEOL JEM 2200FS



2D High-Performance Electronic and Sensing devices



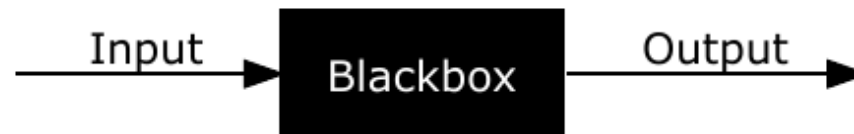
TEM images of TaS3 nanofibers and HR-TEM (D) image of TaS3 with clearly visible (200) and (006) planes.

Electron diffraction of Co-S deposited on Ta substrate

T. Křenek, R. Medlin et al., J. of Alloys and Compounds (2018)

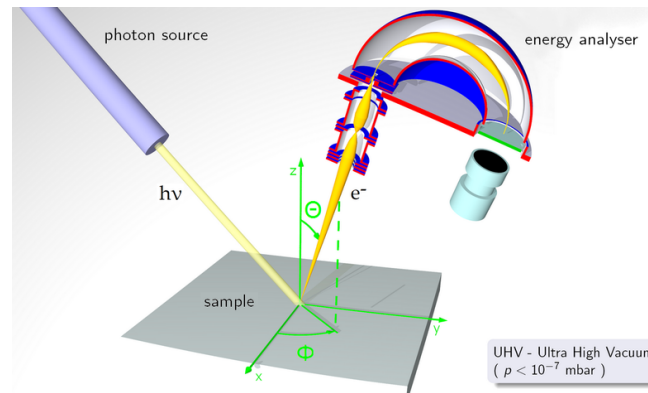
R. Medlin et al., ACS Nano, 12, 464 (2018)

Only indirect methods are available if you want to study interior of a material: blackbox techniques.



Spectroscopy:

Way to investigate ground state of a system by studying its response to a perturbation



Theoretical explanation by A. Einstein (1905):
QUANTIZATION OF LIGHT

Ann. d. Phys. 17, 132 (1905):

Die kinetische Energie solcher Elektronen ist

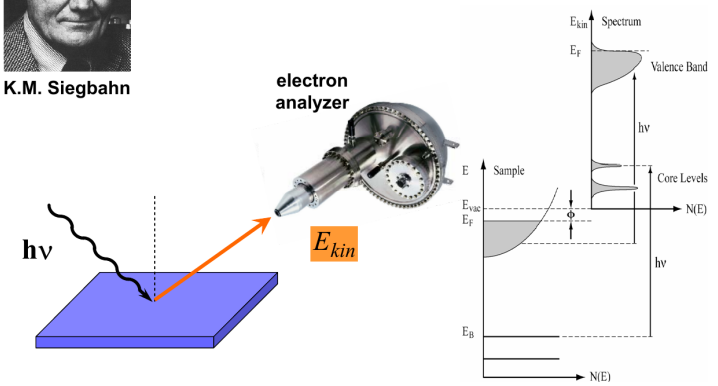
$$\frac{R}{N} \beta \nu - P.$$

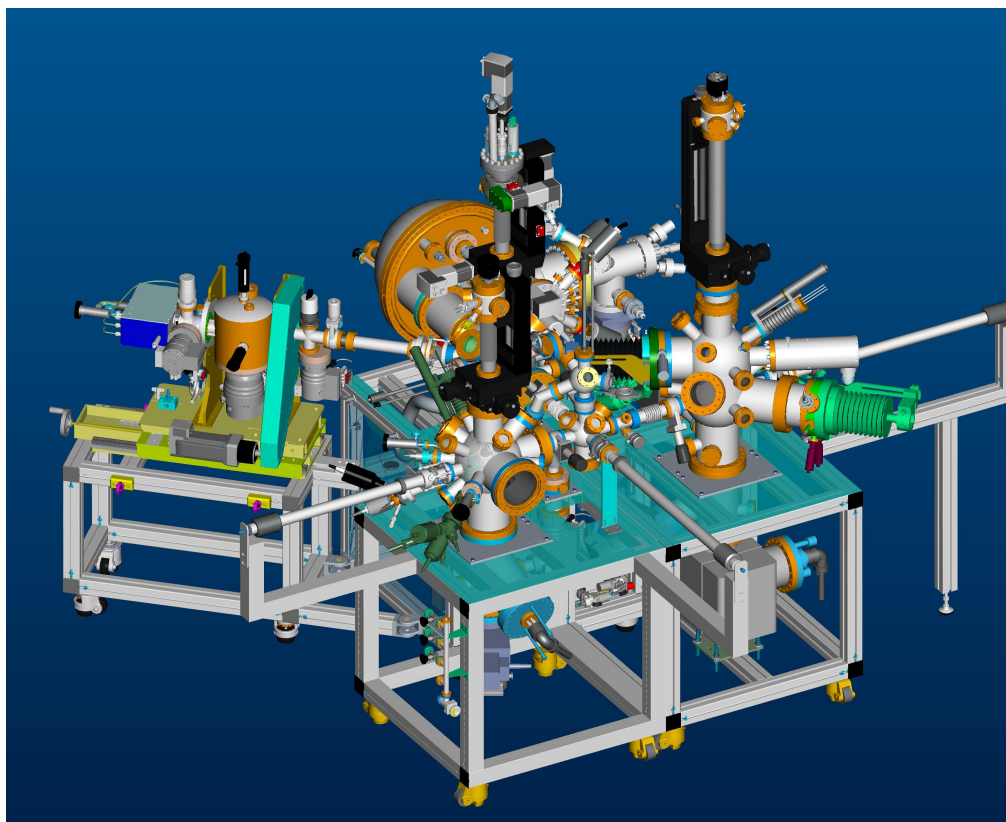
$$E_{kin}^{max} = h \nu - \Phi$$



K.M. Siegbahn

energy conservation: $E_{kin} = h \nu - E_B - \Phi$





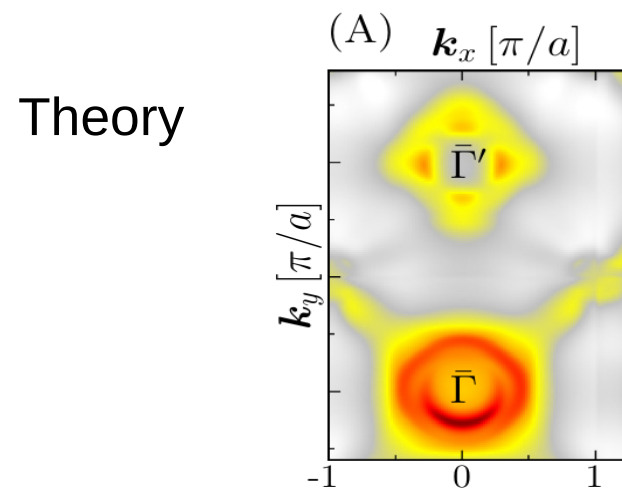
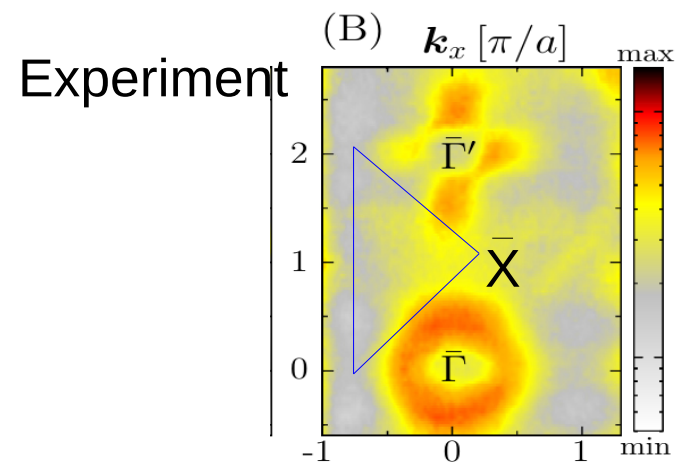
Planned spin resolved ARPES experimental setup
(delivery end of 2018)

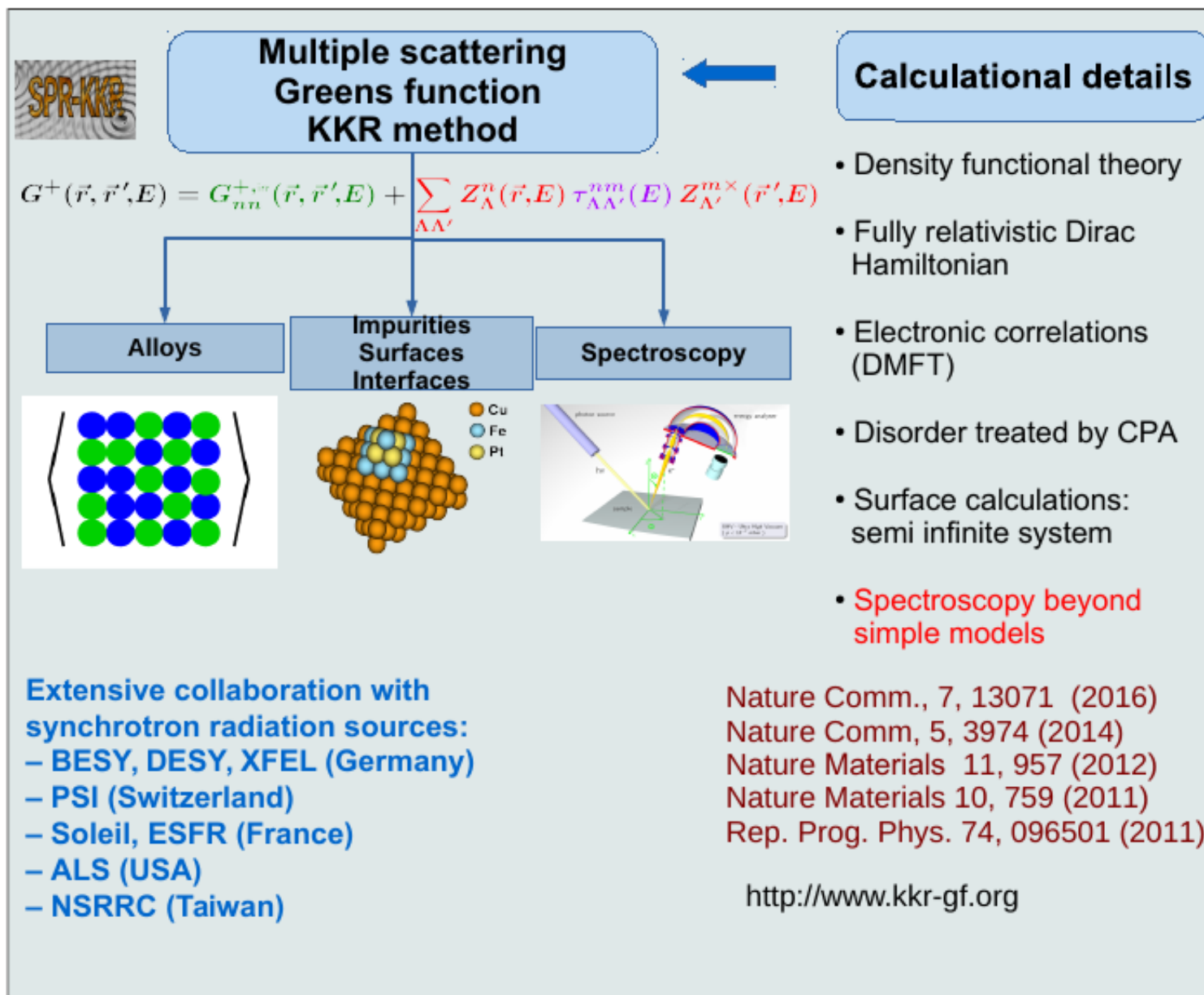
G. Derondeau, S. Polesya, S. Mankovsky, H. Ebert, **JM**, PRB **90**, 184509 (2014)

G. Derondeau, J. Braun, H. Ebert, **JM**, PRB **93**, 144513 (2016)

G. Derondeau, F. Bisti, J. Braun, H. Ebert, M. Kobayashi, M. Shi, V. Strocov and **JM**, Sci. Rep. (2017)

Electronic structure of high Temperature superconductors





- J. Krempasky, H. Dil, V. Strocov, F. Bisti PSI
- J. Fink, Dresden
- K. Hricovini Cergy-Pontoise
- G. Schönhense, H. J. Elmers Universität Mainz
- O. Rader, Bessy, Berlin
- M. Morgenstern: Universität Aachen
- H. J. Elmers: Universität Mainz
- M. Donath, Universität Münster
- C. S. Fadley: University of California Davis
- C. M. Schneider: FZ Jülich
- M. Weinelt, TU Berlin
- F. Parmegiani, Elettra, Trieste
- F. Reinert, H. Bentmann, Universität Würzburg
- H. Ebert, University of Munich
- Ch. Scheu, Max-Planck Institute, Duesseldorf
- K. Hatada, Toyama, Japan
- M. Kobayashi, Tokio, Japan
- ...

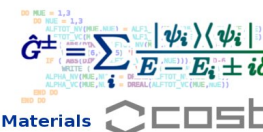
Funding:

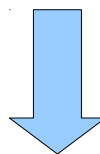


EUROPEAN UNION
European Structural and Investment Funds
Operational Programme Research,
Development and Education

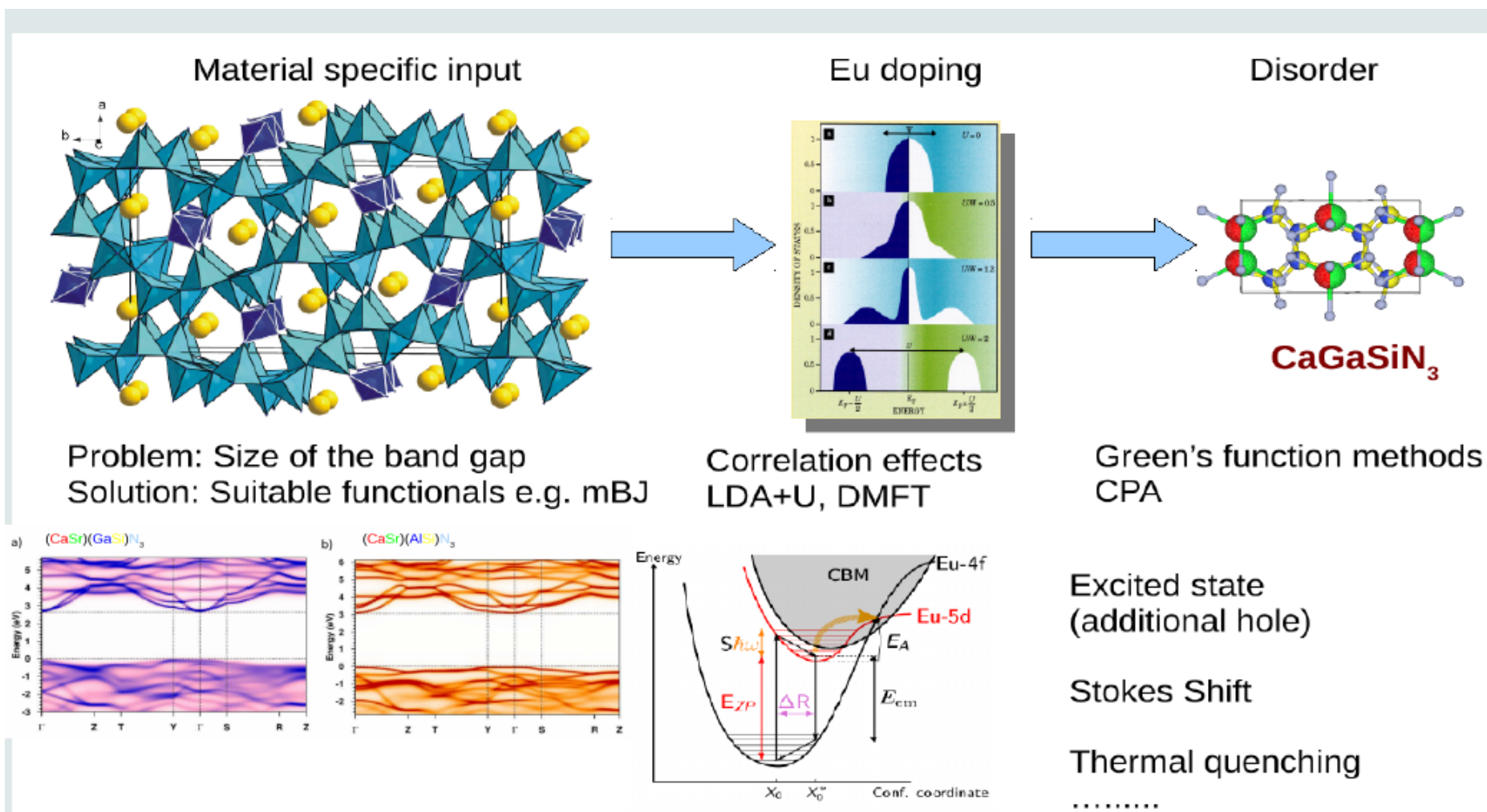


COST Action MP1306:
Modern Tools for
Spectroscopy on Advanced Materials





**Faculty of Sciences, Prof.
Alex Laikhtman**



➡ In collaboration with Prof. Schnick (LMU Munich) and Philips

Phys. Chem. Chem. Phys. 19, 9292 (2017)

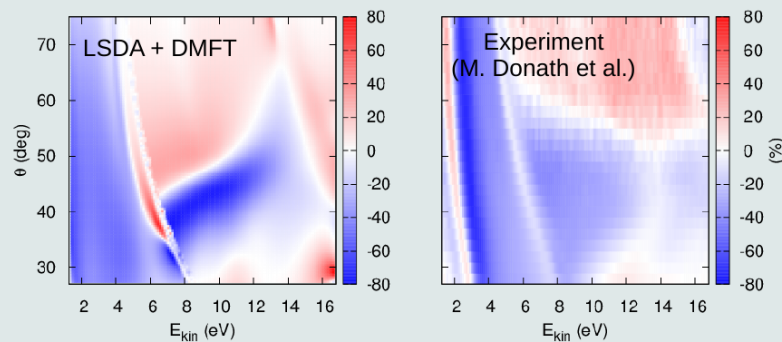


In collaboration with
Prof. Schönhense (Mainz),
Prof. Ebert (Munich)
and SPECS (Berlin)

Spin polarised LEED:

- Search for new materials: O/Fe(001)
- Optimal scattering geometry deduced from theory

SPLEED of (1x1)O/Fe(001)

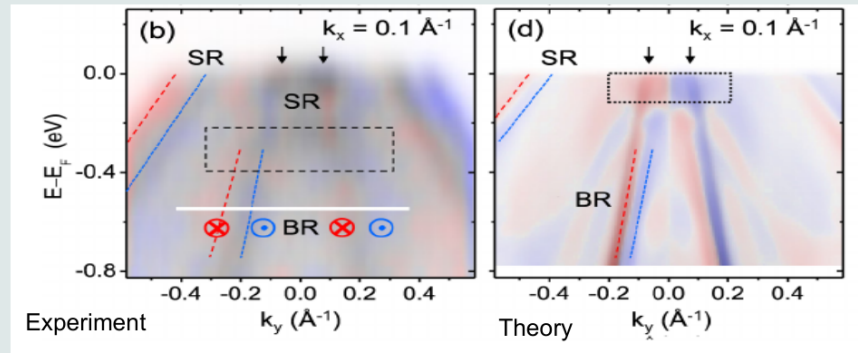


Phys. Rev. B 95, 204423 (2017),
Phys. Rev. B 92, 174408 (2015)

ARPES calculations:

- Test of Performance
- Proof of principle
- Novel materials

ARPES of novel ferroelectric Rashba semiconductors

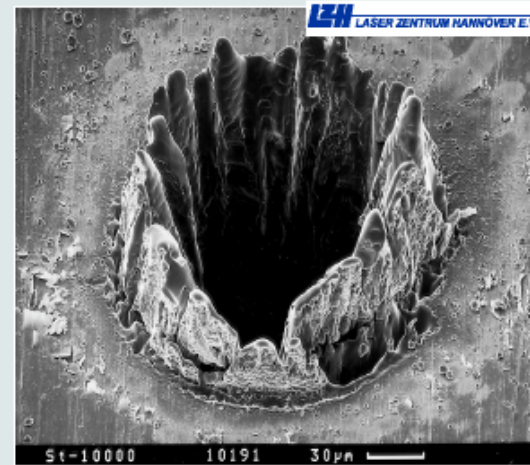
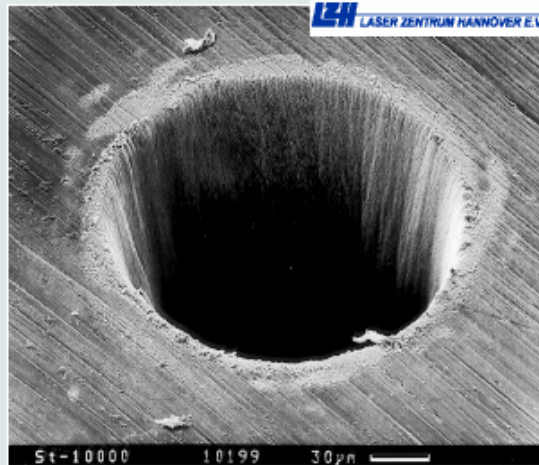


Phys. Rev. B 94, 201403 (2016), 94 205111 (2016)
Nature Scientific Reports 6, 29394,
Nature Comm. 7, 13071 (2016)

Industrially relevant alloys (Stainless Steel FeCrNi)

Laser ablation using ultra-short laser pulses → 3D surface structuring

Steel drilling



2 Temperature Model

Fundamental understanding
of ultrafast interaction
light – matter

$$C_e(T_e) \frac{\partial T_e}{\partial t} = \nabla \cdot [K_e(T_e, T_l) \nabla T_e] - G(T_e)(T_e - T_l) + S$$

$$C_l(T_l) \frac{\partial T_l}{\partial t} = \nabla \cdot [K_l(T_l) \nabla T_l] + G(T_e)(T_e - T_l).$$

Material specific input
from quantum calculations

In collaboration with H. Huber (Munich University of Applied sciences) and



Phys. Rev. B 93, 165119 (2016)