UNIVERSITÄT LEIPZIG

Materials Science and Crystallography
Team of Prof. Dr. Oliver Oeckler

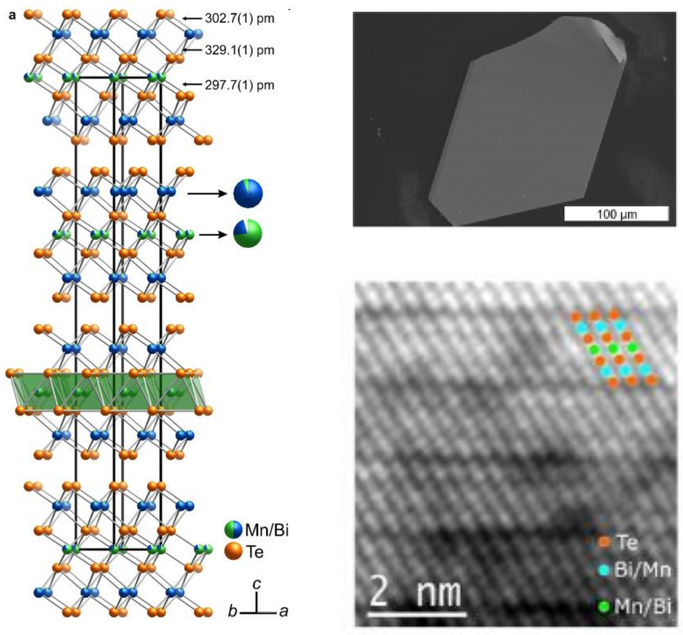
MATERIALS

The group's research focuses on the synthesis, characterization and optimization of a broad range of solid-state compounds:

- thermoelectric materials for waste-heat recovery and cooling
- complex disordered crystals with unusual properties
- rare-earth compounds with charge-density waves, elements in "exotic" oxidation states and mixed anions
- nitride-based luminescence materials e. g. for LED applications
- chalcogenides and pnictides
- cluster compounds

Tellurides as thermoelectric and topological materials

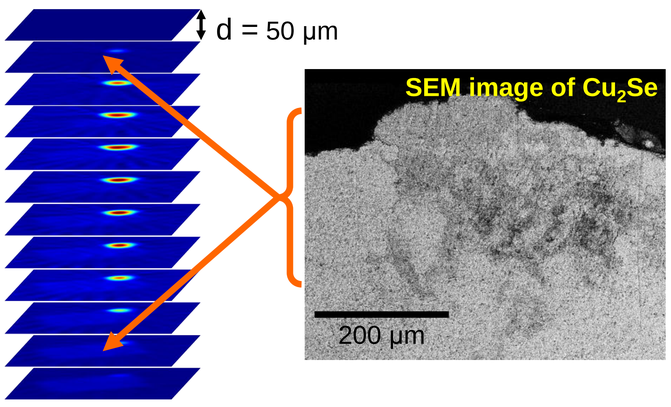
- materials based on GeTe, PbTe, Ge/Sb/Te or Ge/Bi/Te with high thermoelectric performance
- layered structures with intrinsic defects on various length scales
- thermoelectric performance optimized by targeted doping



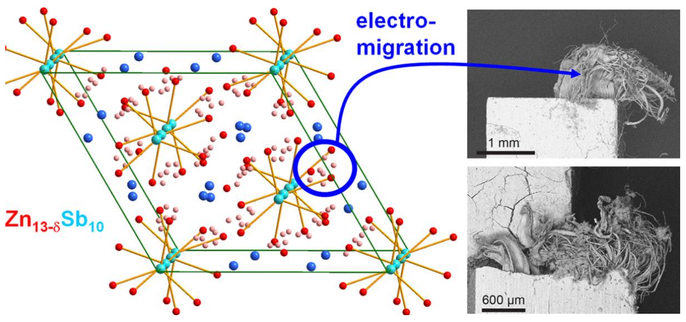
Crystal structure, SEM and HRTEM image of $MnBi_2Te_4$

Stability of high-performance and environment-friendly thermoelectric (composite) materials

- mixed ionic-electronic conductors: $Zn_{13-\delta}Sb_{10}$, Cu_2Se, and $AgCrSe_2$ with high thermoelectric performance, but ionic conductivity leads to decomposition under electrical fields
- X-ray diffraction computed tomography (3D-XRDCT) ***in situ***



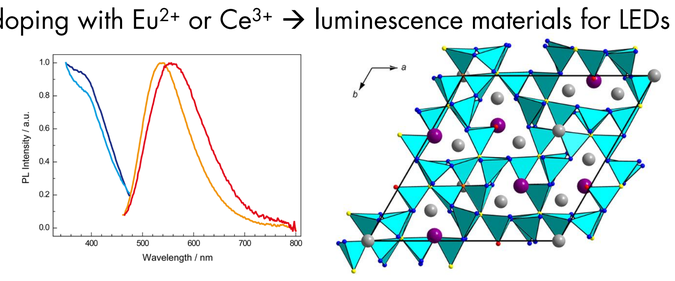
Intensity of a Cu reflection in different layers of the sample (left)



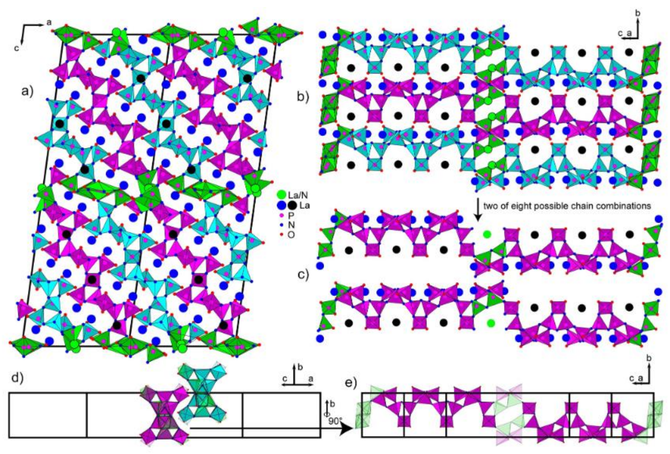
Crystal structure of $Zn_{\sim 12.8}Sb_{10}$
and SEM images of deposited Zn

(Oxo-)Nitridosilicates and -phosphates

- diverse structural chemistry of nitridic frameworks with condensed SiN_4, PN_4, $Si(N,O)_4$ and $P(N,O)_4$ tetrahedra
- doping with Eu^{2+} or Ce^{3+} → luminescence materials for LEDs



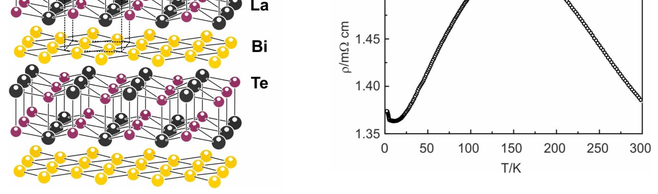
Excitation and photoluminescence spectra and crystal structure of $(Lu/Y)Ba_2[Si_{12}O_2N_{16}C_3]:Eu^{2+}$ with network of $SiC(O/N)_3$ tetrahedra



Complex crystal structure of the oxonitridophosphate $La_{21}P_{40}O_{46}N_{57}$ with highlighted $P(N,O)_4$ network

Charge-density waves (CDW) in rare-earth (*RE*) pnictide chalcogenides *REPnCh* (Dr. C. Benndorf)

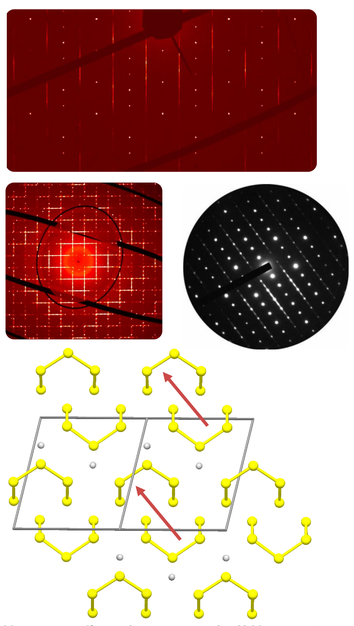
- layered mixed-anionic compounds like *RE*SbS and *RE*BiTe with square-like arrangement of Sb and Bi atoms
- CDWs examined by low-temperature diffraction, electron microscopy and spectroscopy



Crystal structure of LaBiTe and electrical resistivity of NdBiTe indicating CDW formation at 150 K

Complex structures and diffuse scattering

- stacking faults and diffuse scattering of BeP_2 and $BeAs_2$
- structure determination by combination of synchrotron and electron diffraction, bonding analysis with DFT calculations

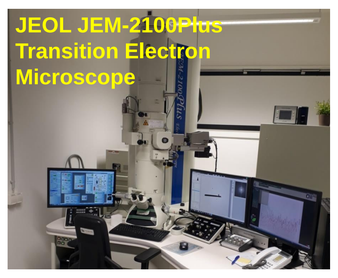


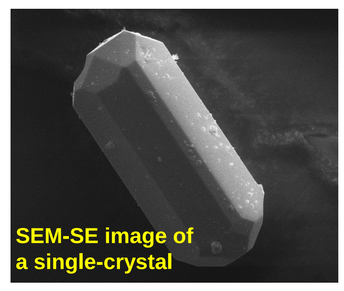
Diffuse reflections and different stacking modes of layers of As_8^{8-} rings in $BeAs_2$

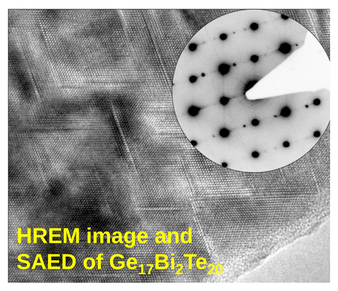
METHODS

Scanning and Transmission Electron Microscopy

- SEM imaging and EDX spectroscopy
  → chemical analysis, microstructure of composite materials
- HRTEM imaging and electron crystallography
  → structure determination of nanocrystals

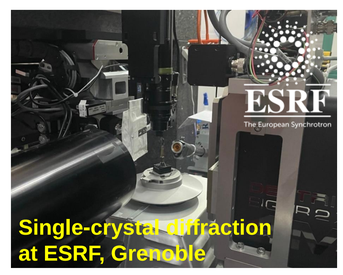


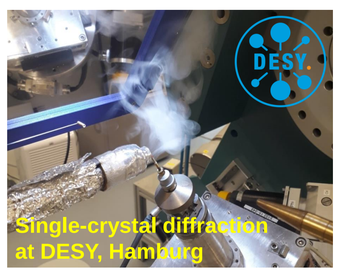




Structure determination → synchrotron methods

- single-crystal and powder diffraction
- micro-focused synchrotron beams → micro-/nano-crystals
- diffuse scattering, resonant diffraction, and more…



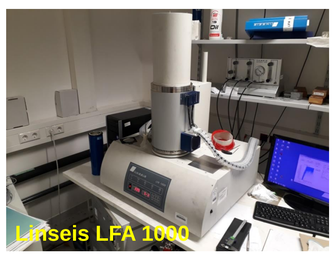


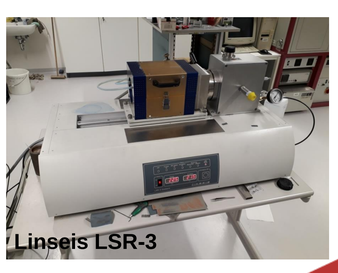
Synthesis

- modern solid-state synthesis: high-temperatures, inert conditions, melt-spinning and high-frequency induction, chemical vapor transport, hydrothermal conditions, flux-assisted synthesis …

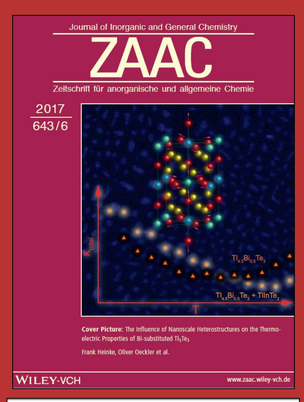
Physical measurements (thermoelectricity)

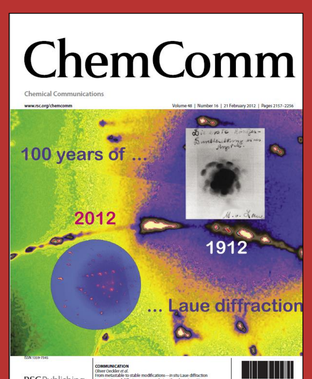
- electrical conductivity and Seebeck coefficient
- thermal conductivity and heat capacity

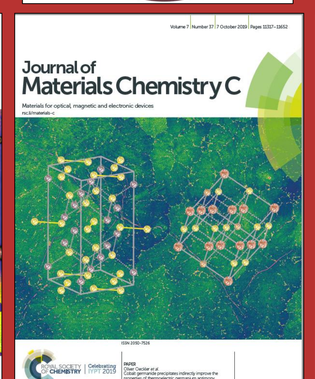


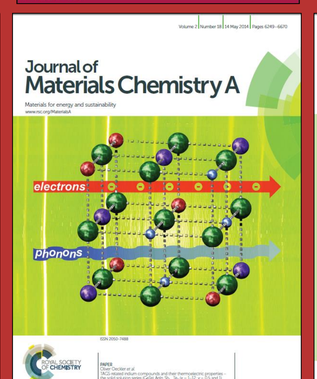


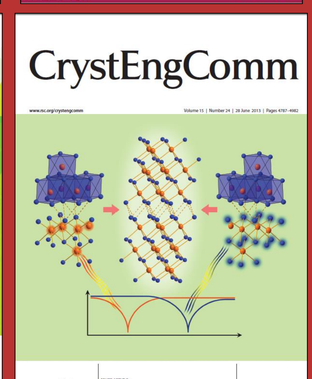
SELECTED PUBLICATIONS











CONTACT

Prof. Dr. Oliver Oeckler
Universität Leipzig
Fakultät für Chemie und Mineralogie
Scharnhorststraße 20, 04275 Leipzig
E-Mail: oliver.oeckler@gmx.de
Tel.: +49 (0) 341 9736251

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