TU Graz

New Energy Materials

An Interdisciplinary Challenge for Research & Innovation

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icTM

OUTLINE

- Intro - General Situation
- Sustainable Energy Systems
  (short survey on advantages & needs)
  - Wind-, Solar-, Geothermic-, Hydro-Power
  - Storage systems
- Materials/Methods/Innovations needed
- Possible Contributions of TU Graz / eseia
  - Some Selected Examples
- Conclusion & Discussion

General Situation
some statements

- Reduction of use of fossil ressources & nuclear energy is an absolute demand !
- Move to renewable ressources → implantable technologies (biomass direct incineration, BtL, BtG, etc.)
- Natural energy ressources wind & sun – not deliverable „on demand“ → Storage necessary
- Different needs for transportation/heating/climati-zation/industry with respect to
  - Capacity,
  - charging speed & infrastructure,
  - Output power

Sustainable Systems
some special demands , selected examples

- **General: restrictions with respect to protection of nature, deep(er) understanding of physics&chemistry, technologies, ...**

  in addition:
  - Wind: availability of / access to mineral ressources (rare earths !!), noise, ice prevention / de-icing
  - Solar: large areas, new materials and systems(textile architecture, low light intensity (dawn), thin film technology, organic materials,
- **Storage / Recovery Systems**
  - Hydropower (protection of nature – caves/underground = expensive);
  - Hydrogen (electrolysis – catalysts/electrodes? – fuel cells)
  - Accumulators/batteries :
    - Safety, new solid state electrolytes
    - Capacity: new electrode materials, alternative renewable ressources (e.g. lignin),
    - Charging technology (fast!! ?) or exchange system (deposite return scheme)

Over All: Interdisciplinary / Multidisciplinary Development Schemes are necessary

Example: organo- electronics, including PV

From History to presence to Future: multidiscipinary approaches:

1980 onwards: Physicists → Theories, Chemists – new Materials („conductive polymers"),

1990s: technology developments – thin films („Nano layers"), structuring technologies (photo-litho etc. towards real „Nanotechnology"

2000s ongoing: nano structuring, self-assembly, additive manufacturing, „molecular technology"

Still necessarry (or even more than ever): collaboration/clustering between chemistry/physics/characterization techniques/production technology/technology/

Some selected Contributions and Examples for the postulated Interactions as found at TU Graz

- Examples, series 1, materials for **Photovoltaics** / Research Group Gregor Trimmel

- Examples, series 2) materials for Energy Storage / Research Group Martin Wilklening

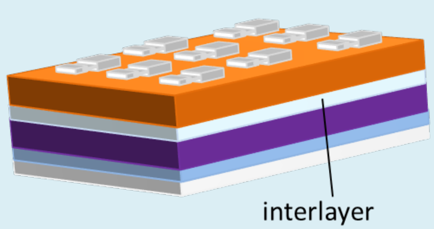
New Materials for photovoltaics

Focus on:

absorber materials processable from solutions (via spin coating, doctor blading etc.)

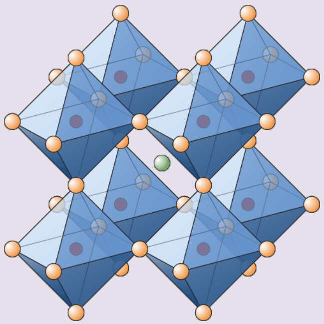
new materials and/or new synthetic approaches

Polymer-NFA (tandem) solar cells



Nanocrystal-polymer solar cells

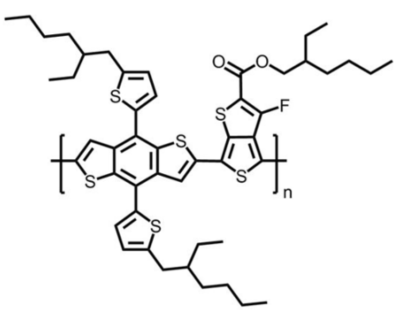
Perovskite solar cells



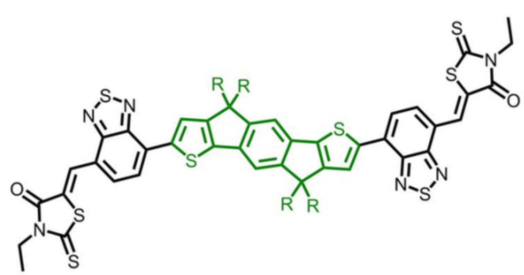
ABX_3

Non fullerene acceptor – polymer solar cells

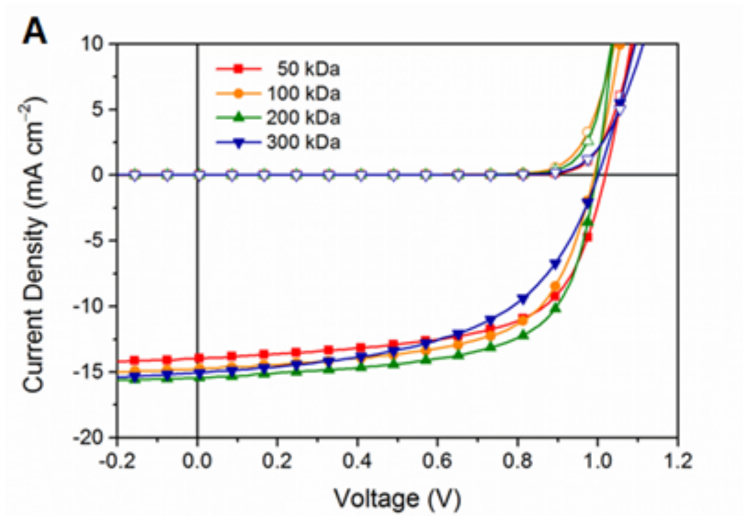
Effect of Polymer Molecular Weight on the Performance of PTB7-Th:O-IDTBR Non-Fullerene Organic Solar Cells



PTB7-Th



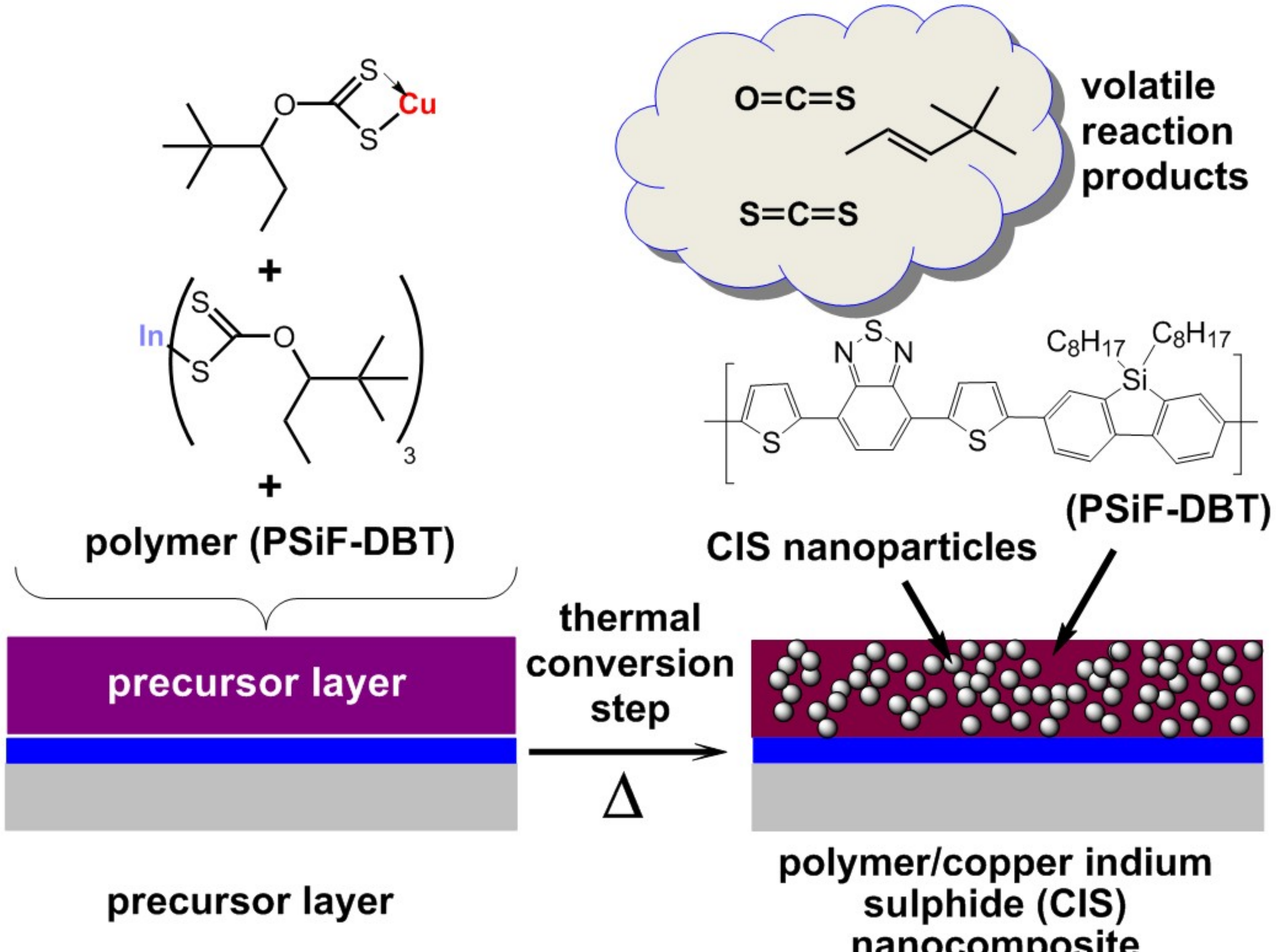
O-IDTBR



Molecular Weight	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)	$EQE_{max.}$ (%)
50 kDa	1.01±0.01	13.5±0.3	62.1±0.6	8.44±0.21 (max. 8.84)	62.4
100 kDa	1.00±0.01	14.2±0.5	61.4±1.4	8.68±0.23 (max. 9.08)	64.1
200 kDa	1.00±0.01	15.2±0.5	63.0±1.6	9.57±0.25 (max. 9.94)	74.9
300 kDa	0.99±0.01	15.1±0.5	51.6±1.3	7.73±0.18 (max. 8.09)	74.0

S. F. Höfler, et al. *J. Mater. Chem. A*, **2018,** DOI: 10.1039/C8TA02467G

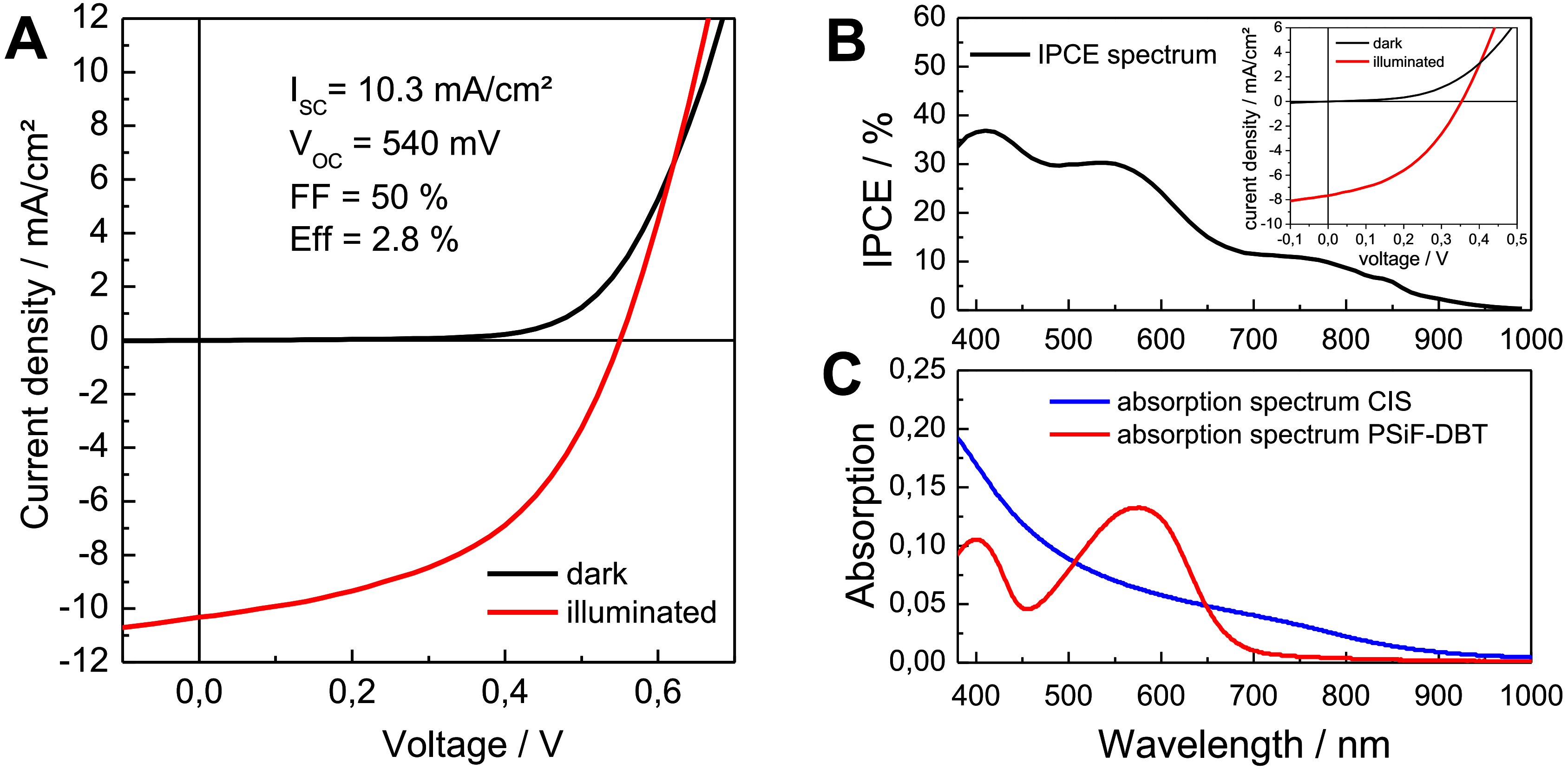
New route to metal sulfide/polymer solar cells



T. Rath et al. Adv. Energy Mater. 2011, 1, 1046

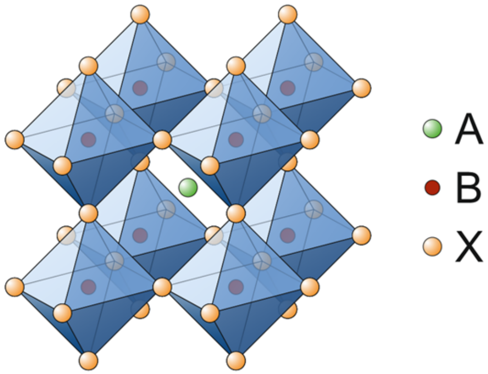
Solar Cells up to 3% efficiency

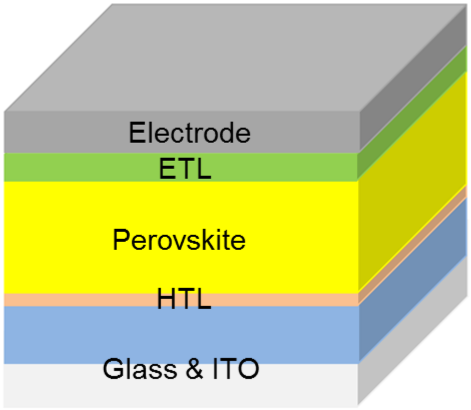
Glass/ITO/PEDOT:PSS/PAL/Al or Ag

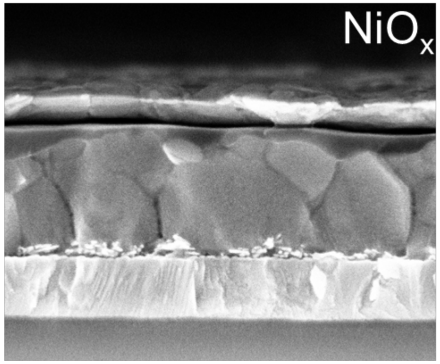


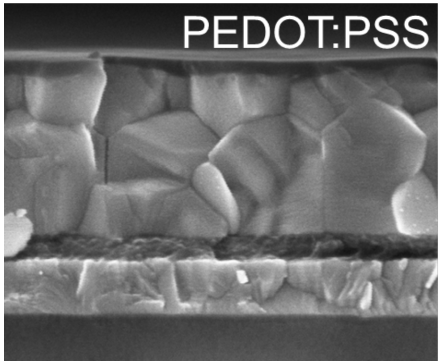
T. Rath et al. Adv. Energy Mater. 2011, 1, 1046

Lead-based Perovskite Solar Cells









A $CH_3NH_3^+$, FA^+, Cs^+
B Pb
C I^-, Br^-

Low temperature processing without TiO_2 which is suitable for preparing flexible solar cells

Substrate/HTLs	V_{OC} (V)	I_{SC} (mA/cm^2)	FF (%)	PCE (%)
NiO_x	0.94	21.73	62.8	12.83
PEDOT:PSS	0.85	18.25	53.8	8.37
MoO_3	0.23	9.84	24.0	0.54
V_2O_5	0.58	3.83	34.3	0.76
no HTL	0.27	15.80	30.8	1.33

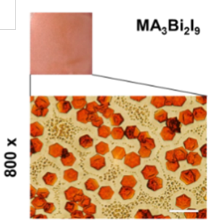
S. Weber, et al. *J. Mater. Sci. Mater. Electron.* **2018,** *29, 1847-1855*

Lead-free Perovskite Materials for Solar Cells

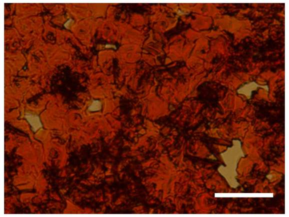
Bismuth-Perovskites

film formation

Standard procedure

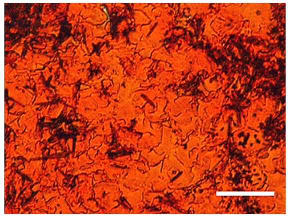


THF drop – modification

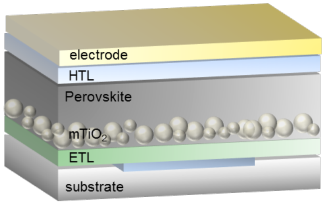


scale bar = 30 µm
magnification: 1000 x

Spin coating of presynthesized MA$_3$Bi$_2$I$_9$ dissolved in THF

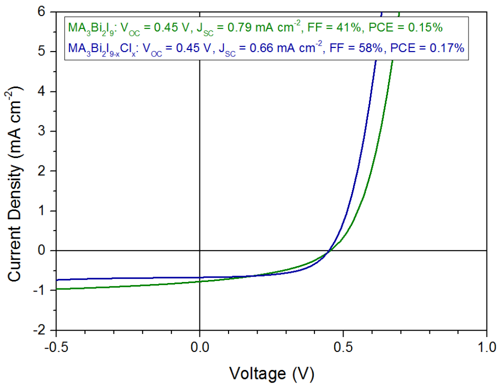


scale bar = 30 µm
magnification: 1000 x



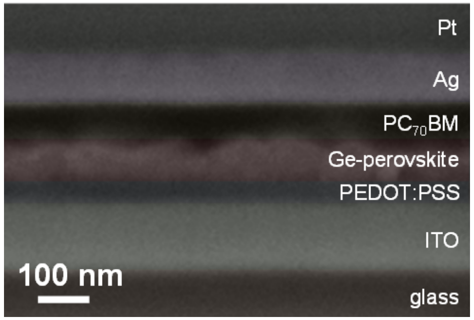
ITO/c-TiO$_2$/mp-TiO$_2$/perovskite/spiro-MeOTAD+TBP+LiTFSI/Au

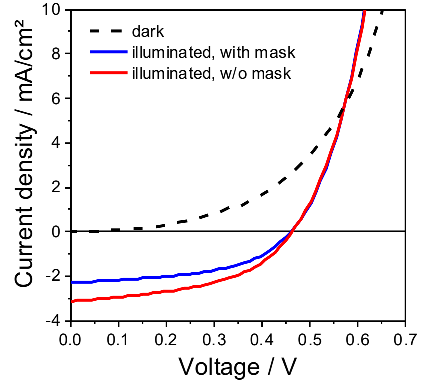
IV-curves

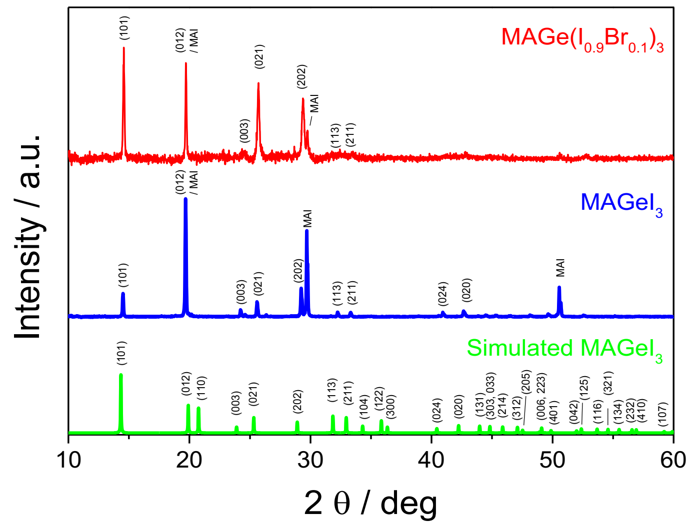


S. F. Höfler, Inorg. Chem. 2019

Germanium-Perovskites







I. Kopacic et al. ACS Appl.Energy Mater. 2018, 1, 343–347

Tin perovskite solar cells

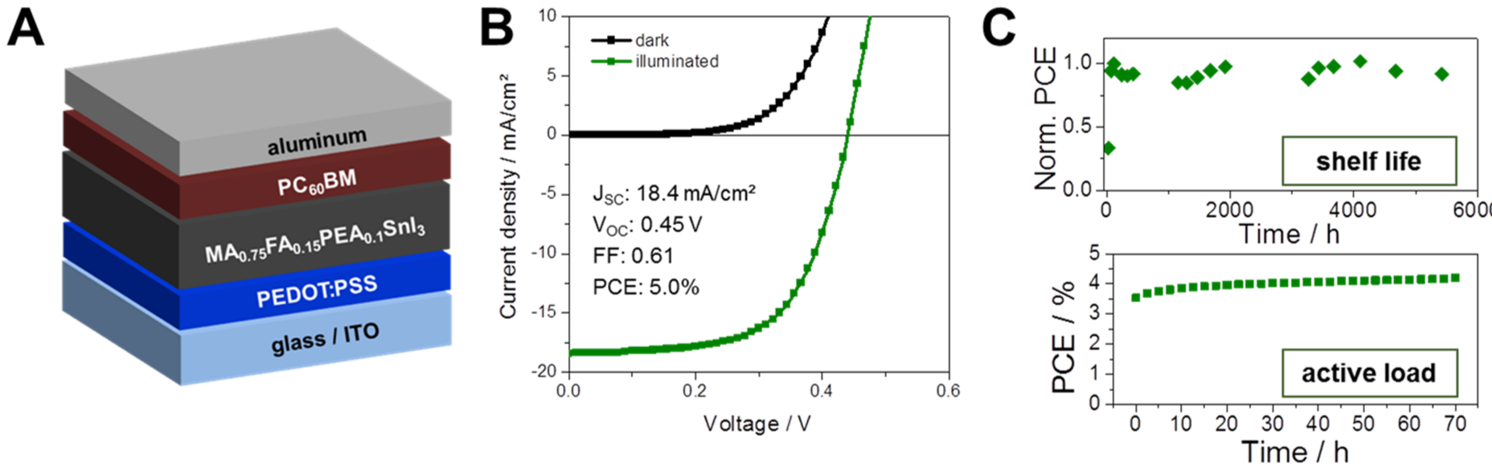
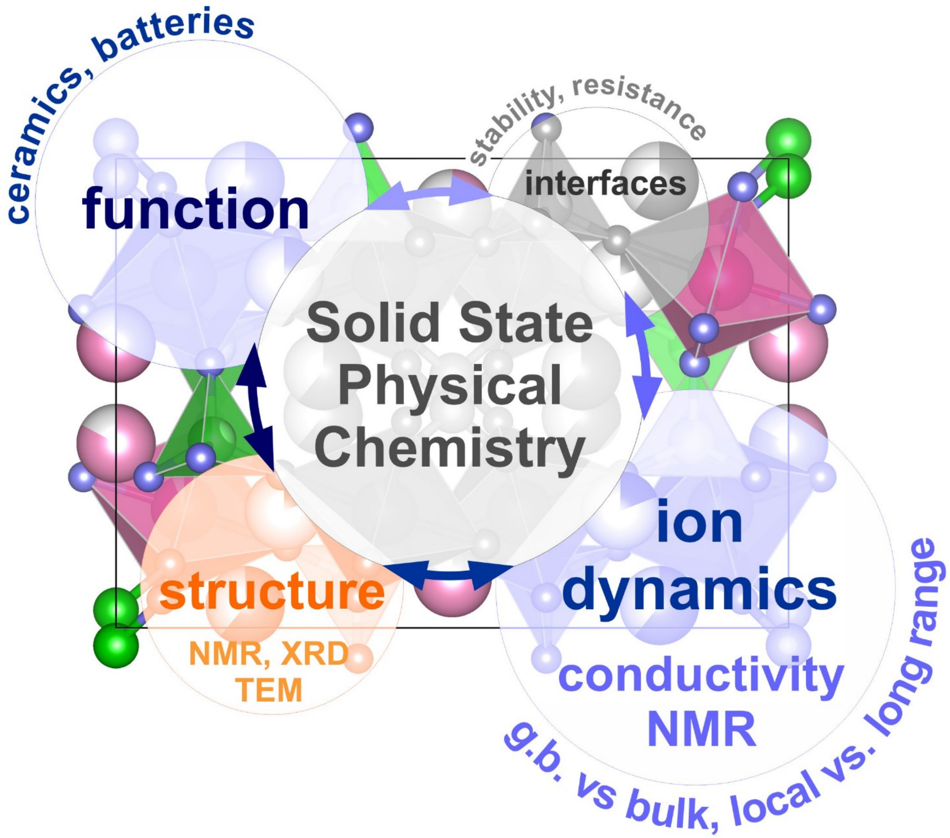


Figure 2: (A) Schematic of the solar cell architecture (B) J-V curves of the tin perovskite solar cell measured in forward scan direction 120 h after fabrication, (C) shelf life time and operational lifetime of these solar cells.

J. Handl, S. Weber, B. Friesenbichler, P. Fürk, T. Dimopoulos, B.Kunert, T. Rath, G.Trimmel, J. Mater. Chem. A 2019,7, 9523-9529

TU Graz / eseia contribution / 2 : Research Group Martin WILKENING

Energy Storage - From Fundamentals to Applications



workgroup Wilkening@ICTM

focusses on the development of sustainable materials

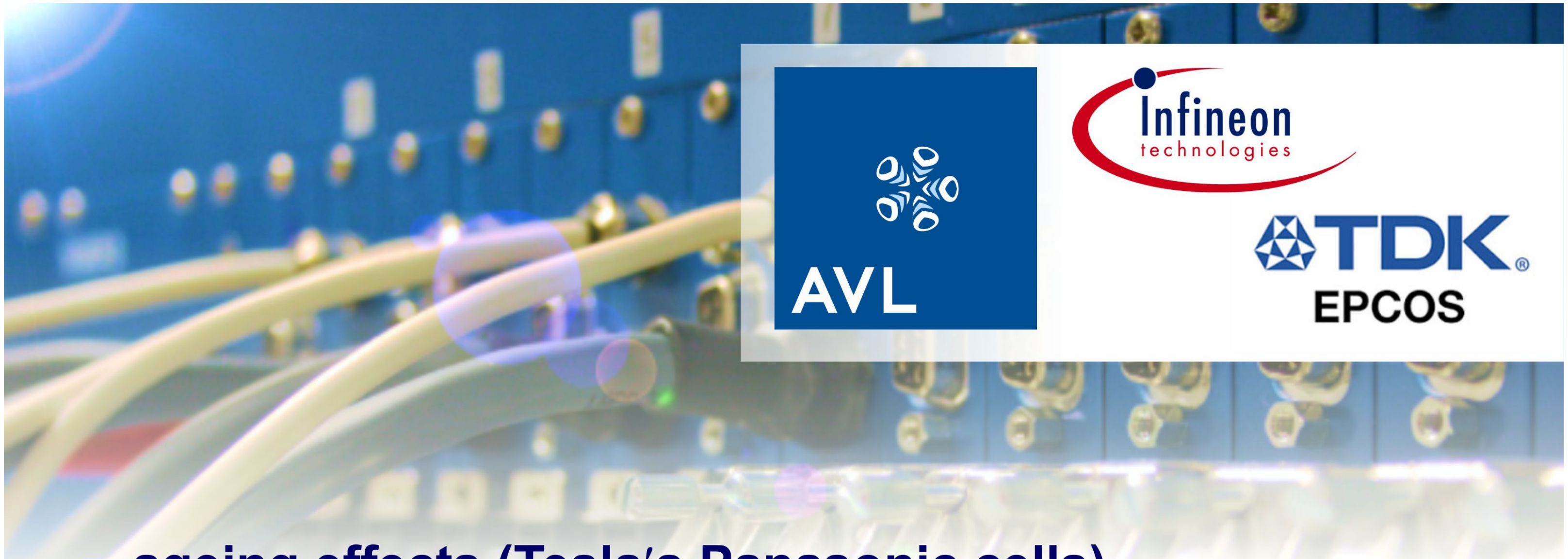
- active materials (anode side)
- solid electrolytes

for battery applications

industrial partners

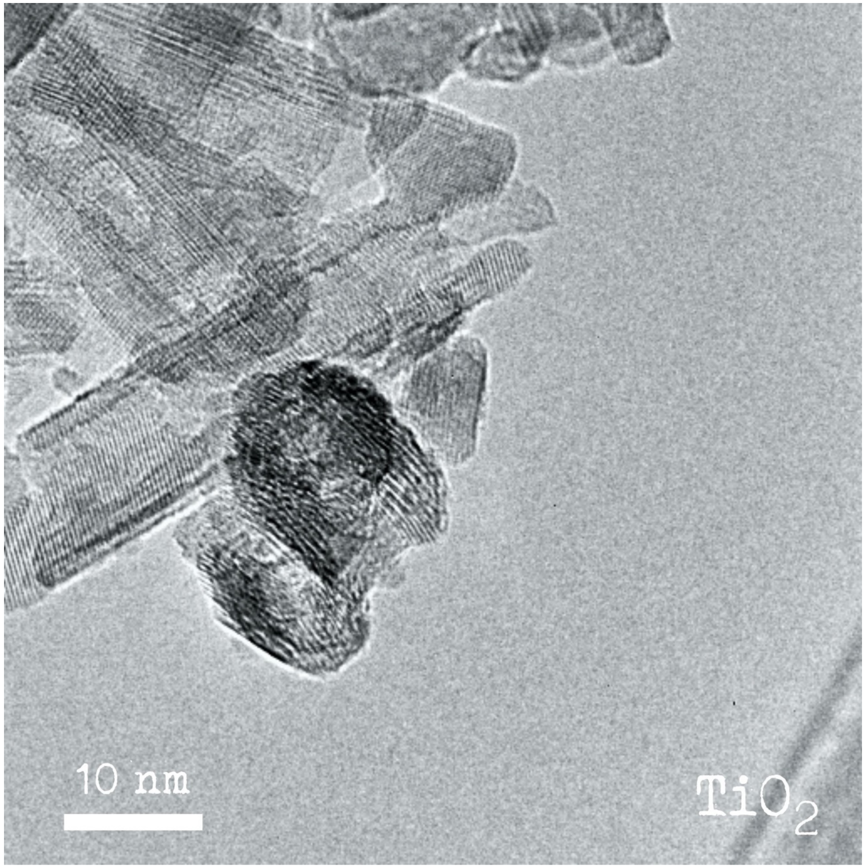
research topics

Christian-Doppler-Laboratory
for Lithium-Batteries



- ageing effects (Tesla′s Panasonic cells), ...
- µ-batteries using single crystalline silicon, ...
- all-solid-state lithium batteries, ...

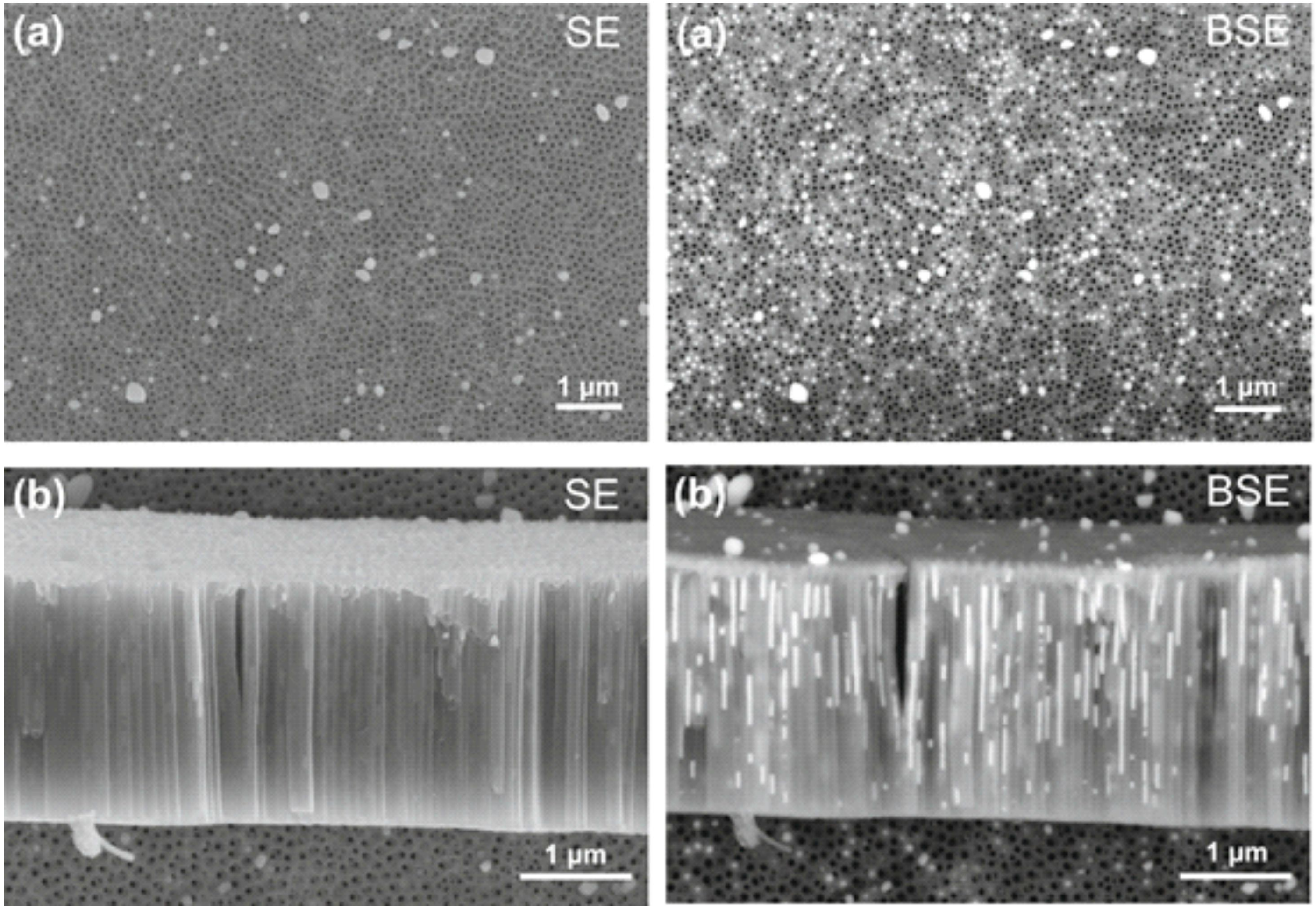
Example 1: nano-titania as anode material



- prepared via hydrothermal techniques in the form of nanotubes
- anodic etching of Ti foil yields amorphous tubes
- useful for both Li and Na batteries.

contact: Dr. Hanzu

nanotubes
of titania
filled with
Sn
(white areas in
BSE mode)



electrochemical
synthesis of anode
materials

Example 2: nano-$LiFePO_4$

DNA-modified

viruses or bacterio-

phages act as

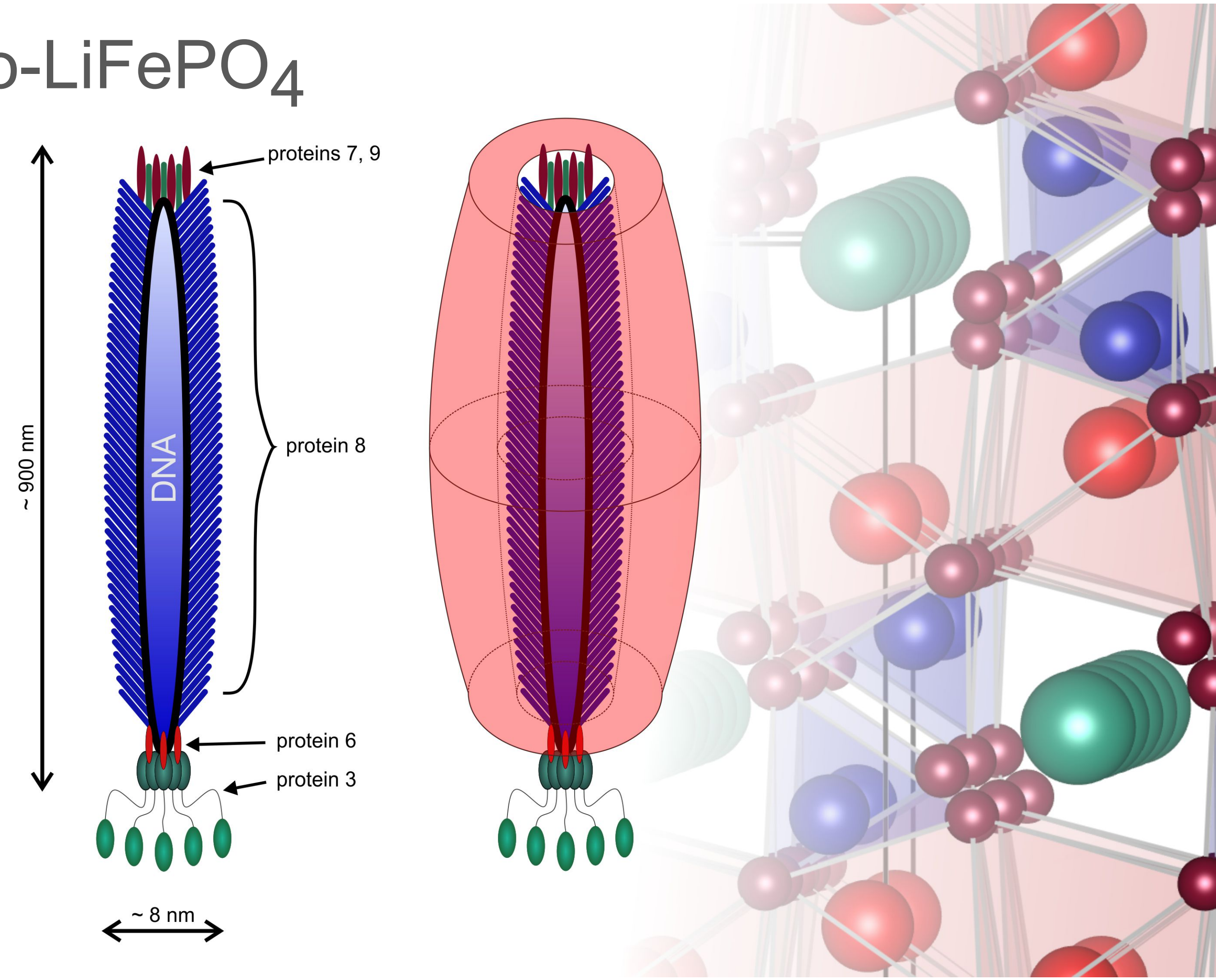
biotemplates

covering

of the bacteriophages

with $LiFePO_4$ from

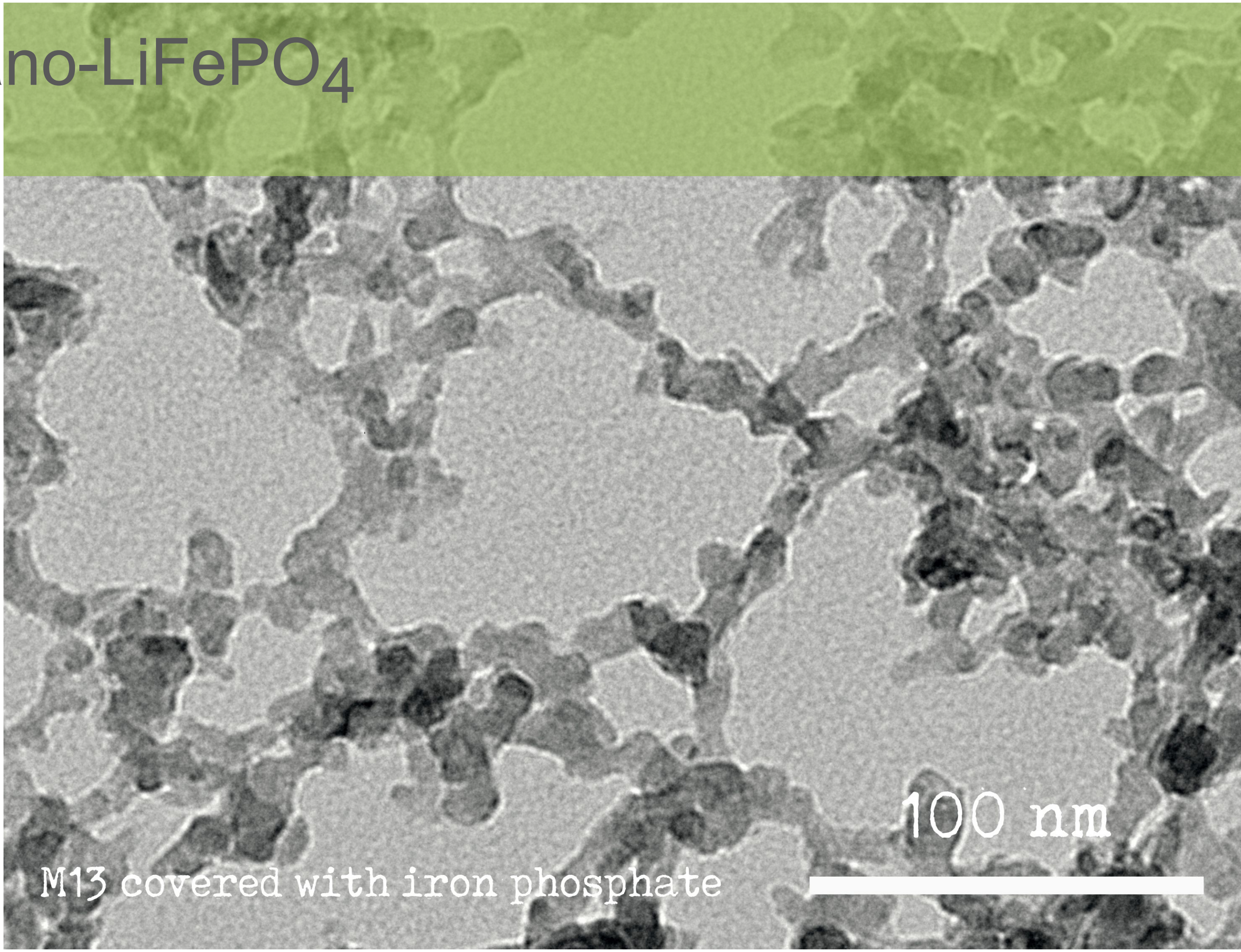
aqueous solution



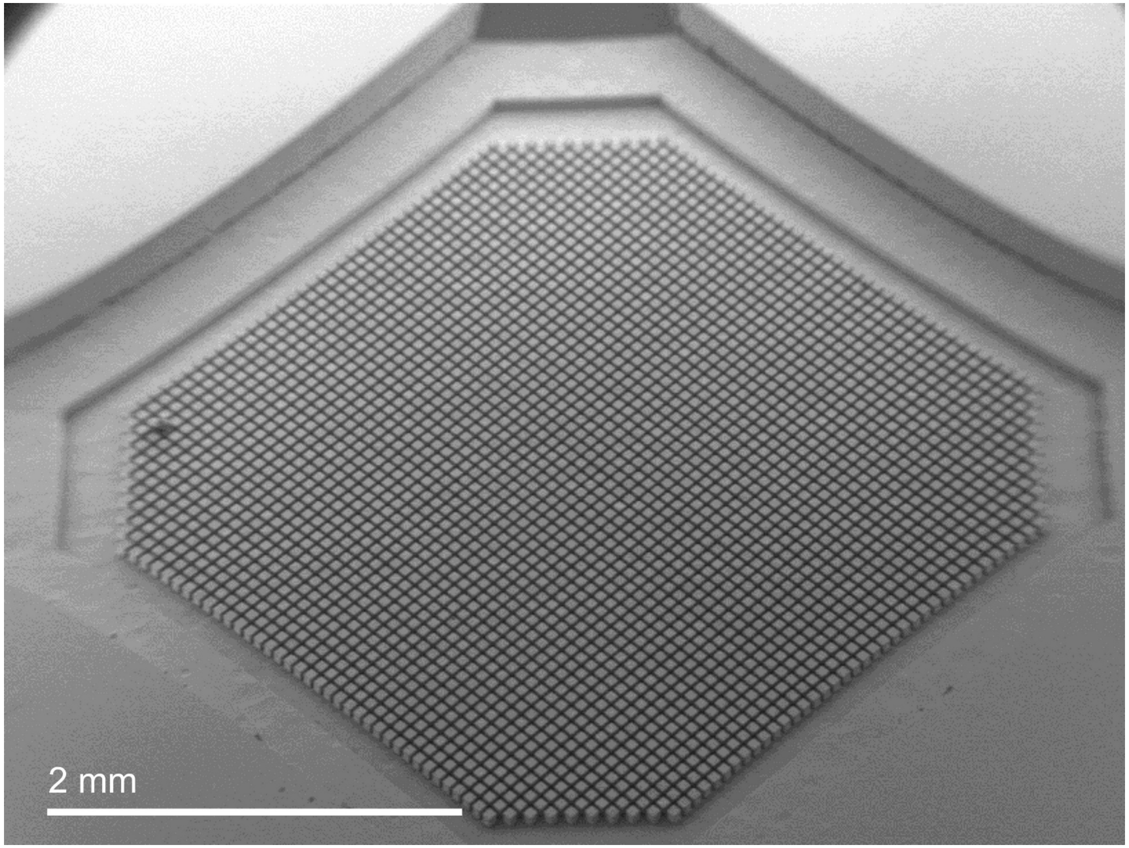
Example 2: nano-$LiFePO_4$

DNA-modified viruses or bacterio-phages act as **biotemplates**

covering of the bacteriophages with $LiFePO_4$ from aqueous solution

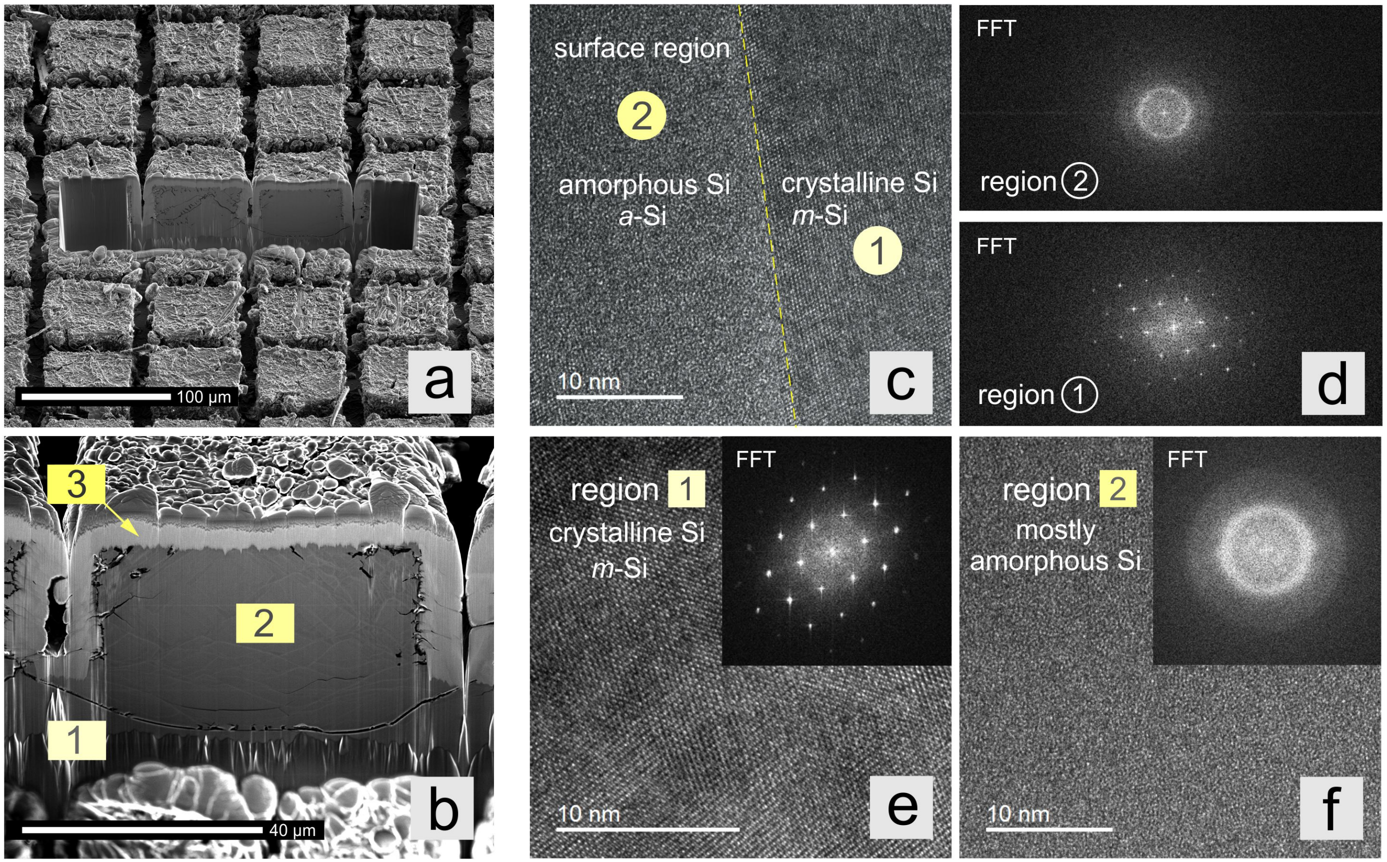


Example 2: Si as anode material in μ-batteries



- monocrystalline Si
- collaboration with Infineon Austria
- structured, 3D-patterned via the BOSCH process
- batteries for the internet of things
- batteries for medicine, smart sensors, RFIDs

Example 2: investigation via SEM and HR-TEM

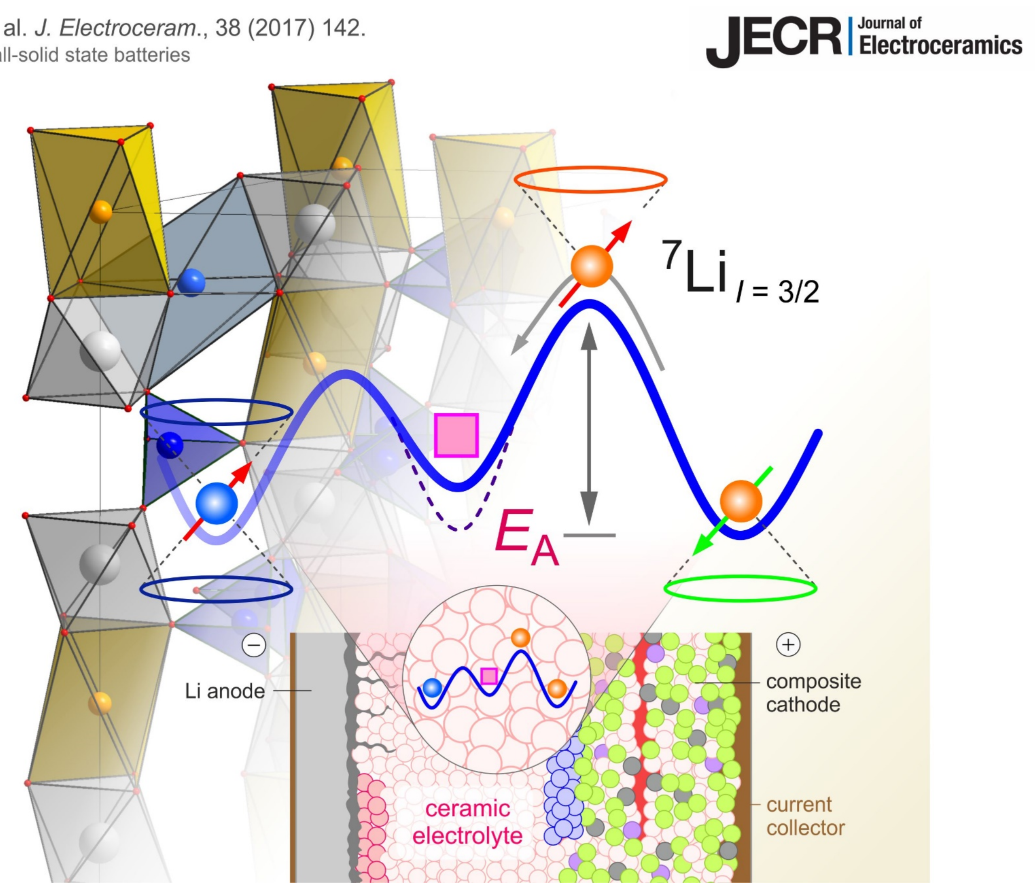


- formation of amorphous LiSi
- investigation of transport parameters via **lithium NMR** at TUG

(USP in Europe)

Example 3: ceramic electrolytes (ion dynamics)

see Uitz et al. *J. Electroceram.*, 38 (2017) 142.
front cover, all-solid state batteries



- micro- and macroscopic Li diffusion parameters
- NMR, broadband impedance spectroscopy

cooperation partners:

QENS, EXAFS, positron annihilation, beta-NMR, neutron diffraction, etc.

Materials: selection

- **LATP: bulk vs. g.b.**

  PCCP,
  J. Mater. Chem.

  lithium alumium phosphates
  Li(7) spin-lock NMR
  low *T* broadband conductivity spectr.

- **garnets: LLZO-based**

  Chem. Mater.
  Inorg. Chem.

  LLZMO, Mo on Zr sites
  LLZTO, Ta on Zr sites, single crystal
  Al-/Ga-bearing LLZO

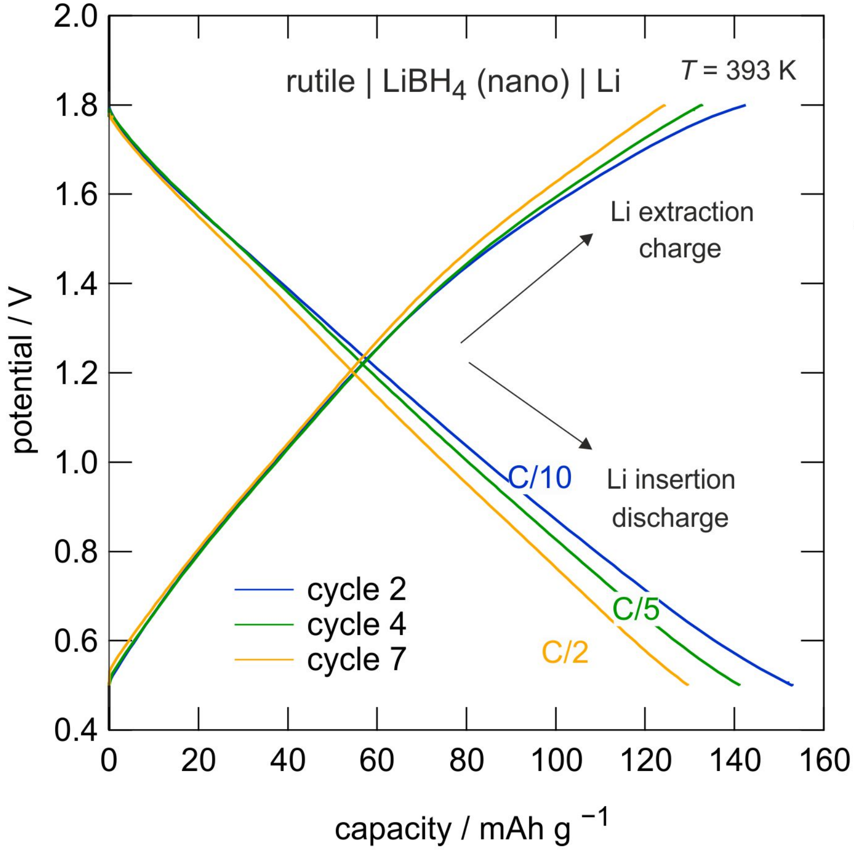
- **thiophosphates argyrodites**

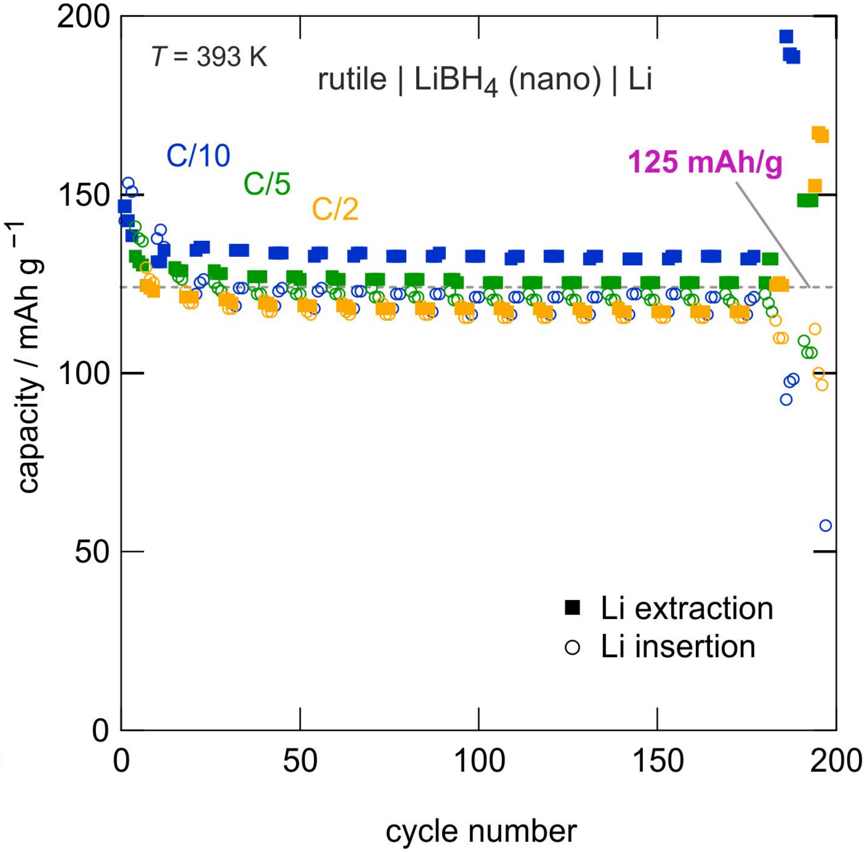
  J. Phys. Chem. Lett.
  ChemPhysChem
  J. Phys. Chem. C

  Li-7-P-11 phase, $Li_7P_3S_{11}$
  γ- and β-Li_3PS_4

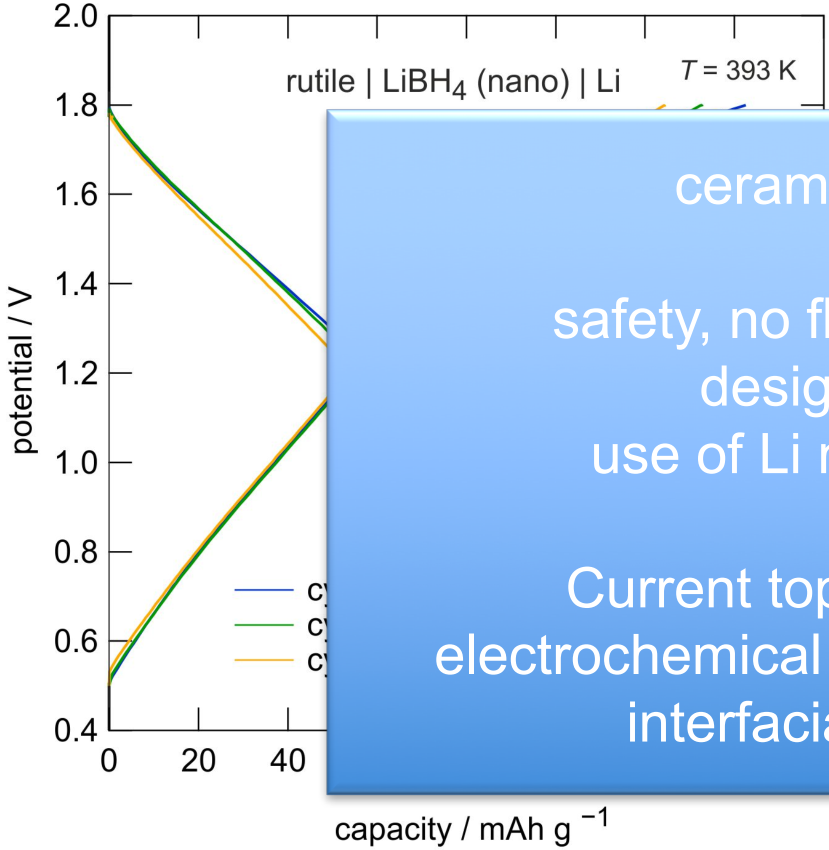
ion dynamics

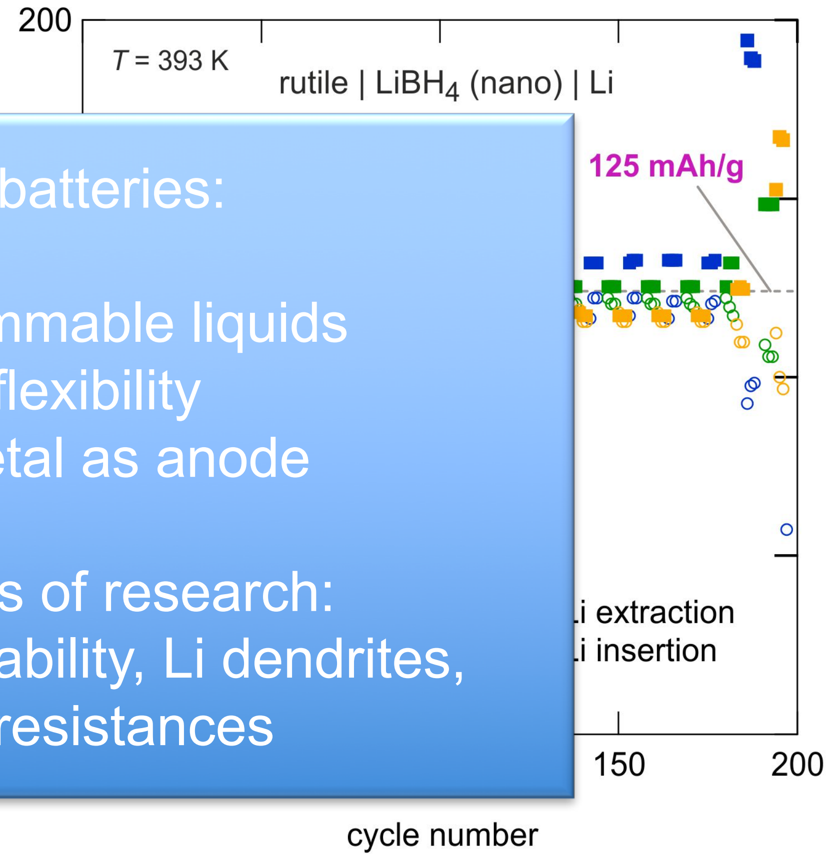
Example 3: titania as anode in all-solid-state batteries





Example 3: titania as anode in all-solid-state batteries





ceramic batteries:

safety, no flammable liquids
design flexibility
use of Li metal as anode

Current topics of research:
electrochemical stability, Li dendrites,
interfacial resistances

Take Home Message:

Development of „Energy Materials“

- Has not yet reached its peak
- Only possible by intensive **inter- /multi-disciplinary/ multinational collaboration**
- Needs
  - **sustainable ressources**
  - **sustainable infrastructure**
  - **Intensive collaboration between science and application (industry) with strong funding at low TRLs**