Achievements of Prof. J. Molenda

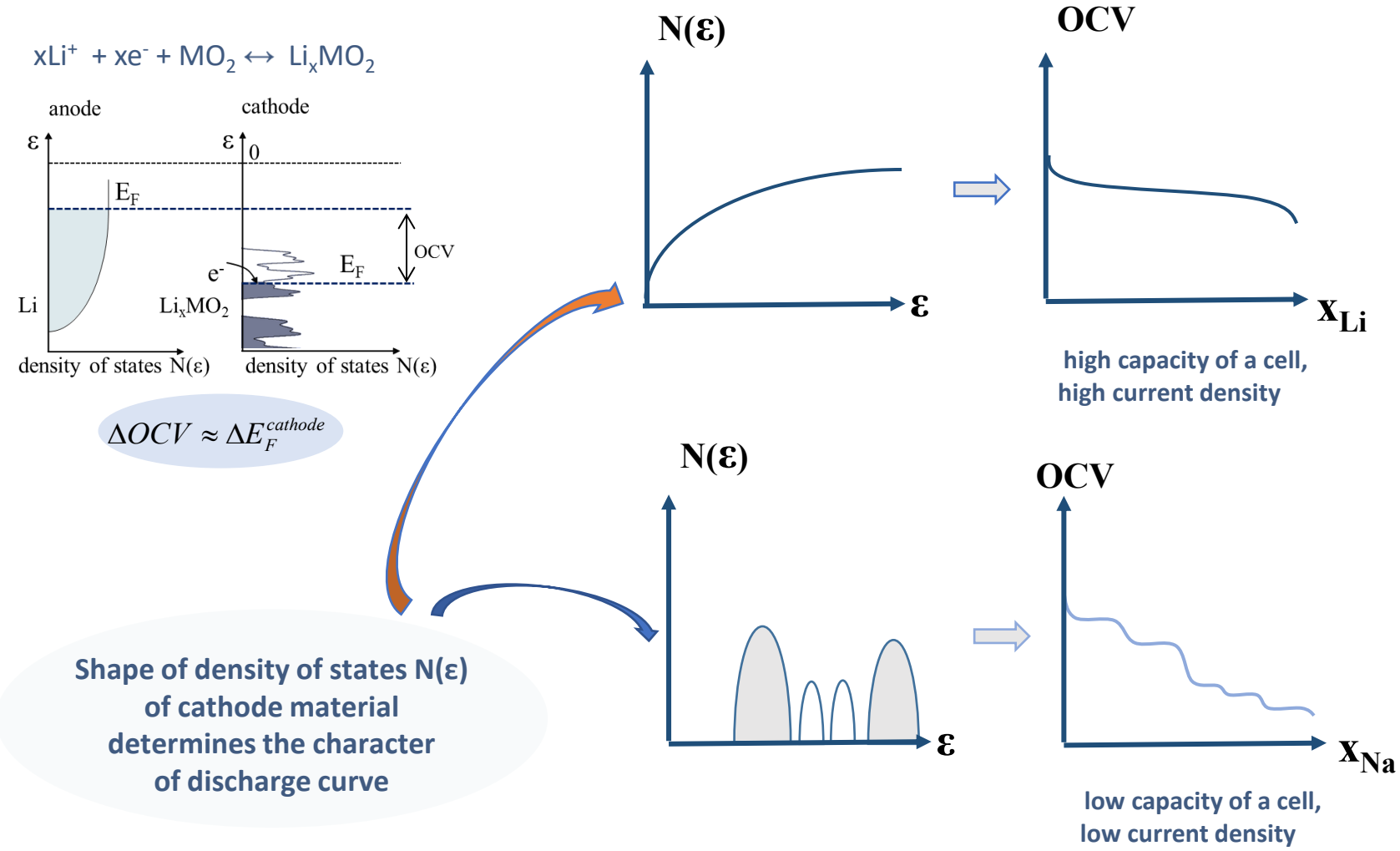
Prof. Janina Molenda – expert in the area of disign and development of functional materials and processes for lithium and sodium batteries technology

- Co- founder and President of Polish Consortium of Electrochemical Energy Storage – PolStorEn (2020-2022)
- Co-founder and President of Polish Hydrogen and Fuel Cells Association (http://www.hydrogen.edu.pl) since 2004
- Head of the Departament of Hydrogen Energy Faculty of Energy and Fuel AGH (2009-2024)

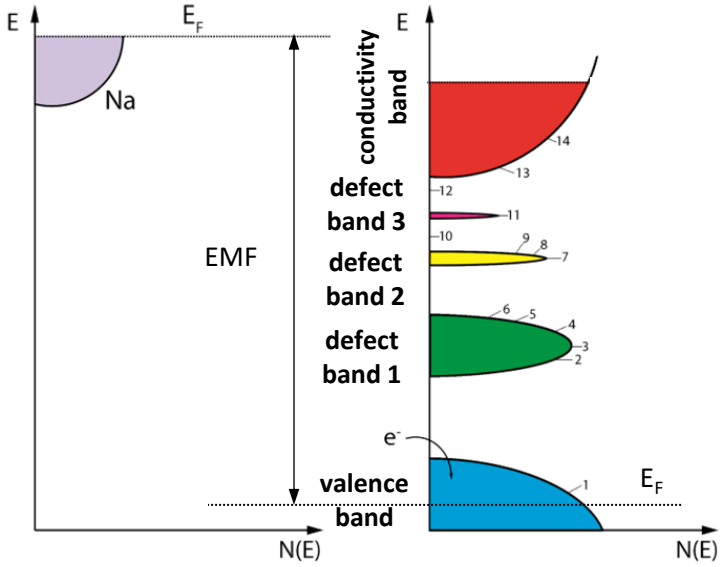
- Prof. J. Molenda is the author of over 170 scientific publications from IF in the area of lithium and sodium batteries, 5 chapters in research book and 7 patent applications (http://home.agh.edu.pl/~molenda). H-index 34, total citations 4 346 (Scopus)
- Prof. J. Molenda has promoted 20 doctors from the area of lithium and sodium batteriess
- Principal investigator on over 30 research projects in the field of lithium and sodium batteries (international, KBN, NCN):
  - UE: New generation of Li-ion batteries with conducting phosphoolivine, UDAPOIG. 01.01.0200108/0901
  - Swiss: Positive Electrode Materials for Li-ion Batteries for Electric Vehicles Application (LiBEV)
  - Singapore: Investigation, Development and Applications of Rechargeable Thin Film Microbatteries for Microelectronics
- Prof. J. Molenda is the organizer of biennial international conferences SMART ENERGY CONVERSION AND STORAGE

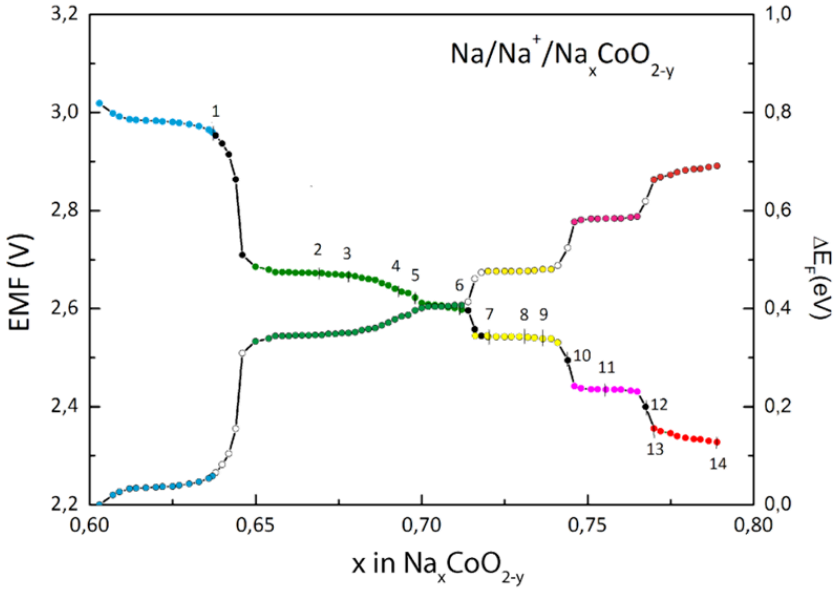
Prof. Janina Molenda proposition:

„Electronic structure engineering” as a new tool in development of functional electrode materials for Li-ion and Na-ion batteries



Works of J. Molenda on the Na_xCoO_{2-y} system clearly document that the step-like character of the discharge curve of the Na / Na^+ / Na_xCoO_{2-y} cell, which arouses controversy in world literature, is purely electronic in nature and reflects abrupt changes in the location of the Fermi level in the anomalous Na_xCoO_{2-y} electronic structure induced by oxygen nonstoistoichiometry.





M. Rybski, J. Tobola, S. Kaprzyk, J. Molenda, Solid State Ionics, 321 (2018) 23
J. Molenda et al., Phys. Chem. Chem. Phys., 19 (2017) 25697
J. Molenda et al., Solid State Ionics 271 (2015) 15
J. Molenda et al., Solid State Ionics 268 (2014) 179
J. Molenda et al., Funct. Mater. Lett. 7 (2014) 1440009
J. Molenda et al., Phys. Chem. Chem. Phys. 16 (2014) 14845

On-going materials studies

Electrode materials for **Li-ion batteries**:

Cathode materials:

- $LiFePO_4$
- Layered oxides:
  - ✓ $LiNi_{1-y-z}Co_yMn_zO_2$
  - ✓ $LiNi_{1-y-z-d}Co_yMn_zCu_dO_2$
  - ✓ $LiNi_{1-y-z-d}Co_yMn_zTi_dO_2$
  - ✓ $LiNi_{1-y-z-d}Co_yMn_zAl_dO_2$
- Li-rich cathodes $Li[Li_yMn_{1-y-2z}Ni_zCo_z]O_2$
- High entropy oxides:
  - ✓ $Li_xMn_{1/4}Fe_{1/4}Co_{1/4}Ni_{1/4}O_2$
  - ✓ $Li_xMn_{1/5}Fe_{1/5}Co_{1/5}Ni_{1/5}Cu_{1/5}O_2$

Anode materials:

- $Li_4Ti_5O_{12}$

Electrolytes:

- $La_{2/3-x}Li_{3x}TiO_3$
- $Li_7La_3Zr_2O_{12}$
- $LiTi_2(PO_4)_3$
- Composites electrolytes:

Ceramice solid electrolyte/PEO

Electrode materials **Na-ion batteries**:

Cathode materials:

- Layered oxides:
  - ✓ $Na_xMn_{1-y}Mg_yO_2$
  - ✓ $Na_xCo_{1-y}Mn_yO_2$
  - ✓ $Na_xCo_{1-y}Fe_yO_2$
  - ✓ $Na_xFe_{1-y}Mn_yO_2$
  - ✓ $Na_xCo_{1/3}Ni_{1/3}Mn_{1/3}O_2$
  - ✓ $Na_xCo_{1-y-z}Ni_yMn_zO_2$
  - ✓ $Na_xNi_{1/3}Mn_{2/3-w}Ti_wO_2$
  - ✓ $Na_xNi_{1-y-z-w}Fe_yMn_zCu_wO_2$
- High entropy oxides:
  - ✓ $Na_xMn_{1/5}Fe_{1/5}Co_{1/5}Ni_{1/5}M_{1/5}O_2$
  - ✓ $Na_xMn_{1/6}Fe_{1/6}Co_{1/6}Ni_{1/6}Cu_{1/6}M_{1/6}O_2$
- Polyanion compounds:
  - ✓ $Na_xFe_2(SO_4)_3$
  - ✓ $Na_3Fe_2(PO_4)_3$, $Na_2Fe_3(PO_4)_3$

  Prussian Blue Analogues

Anode materials:

- MoS_2
- $MoSe_2$
- MoO_3
- $Na_xFe_xTi_{1-x}O_4$ (x=0.9, 0.8)
- $Na_{0.66}Li_{0.22}Ti_{0.78}O_2$
- $Na_2Ti_3O_7$
- Sb/Sb4O5Cl2/C

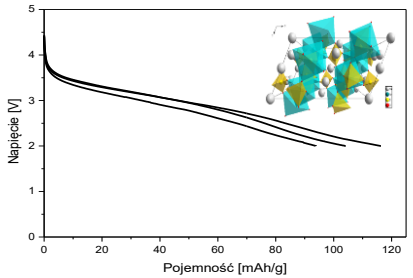
Electrolytes:

- $Na_3Zr_2Si_2PO_{12}$

How to achieve in Na-ion technology energy density levels of commercial Li-ion batteries?

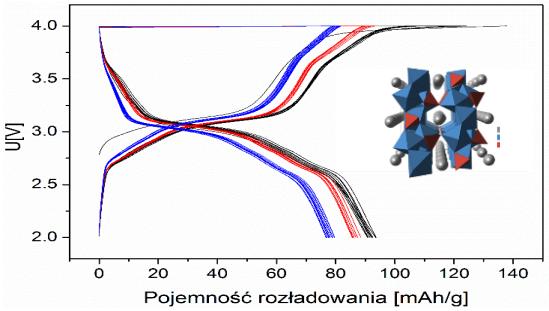
Our proposition of Co-free cathode materials for Na-ion batteries: polyanion compounds and layered oxides with high potential and relatively high capacity

$Na_2Fe_2(SO_4)_3$



simple synthesis
in water environment at 100°C, capacity near theoretical value
120 mAh/g and 450 mAh/l
Patent pending

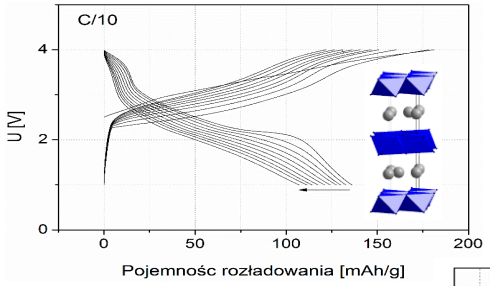
$Na_{2-x}Fe_3(PO_4)_3$



temp. of synthesis 550°C, capacity
100 mAh/g and 400 mAh/l

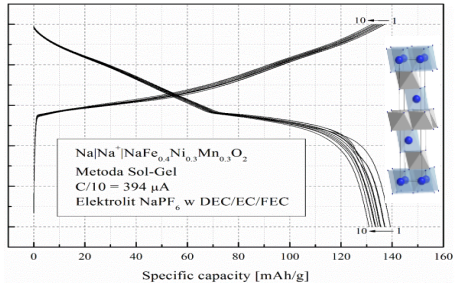
Eco-friendly elements: **Na, Fe, Mn, Ni, S, P,**

$Na_xFe_yMn_{1-y}O_2$



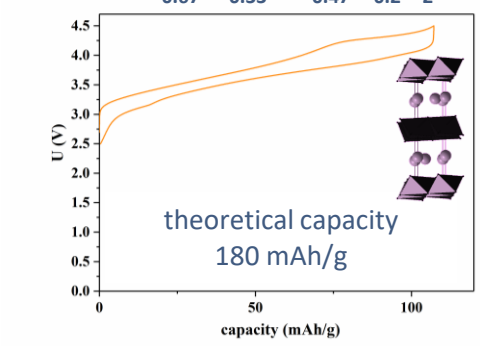
solid state synthesis,
capacity 120 mAh/g
(theoret. 270 mAh/g and 600 mAh/l)

$NaFe_y(Mn_{0.5}Ni_{0.5})_{1-y}O_2$



capacity 140 mAh/g (theoret. 270 mAh/g and 600 mAh/l)

$Na_{0.67}Ni_{0.33}Mn_{0.47}Ti_{0.2}O_2$



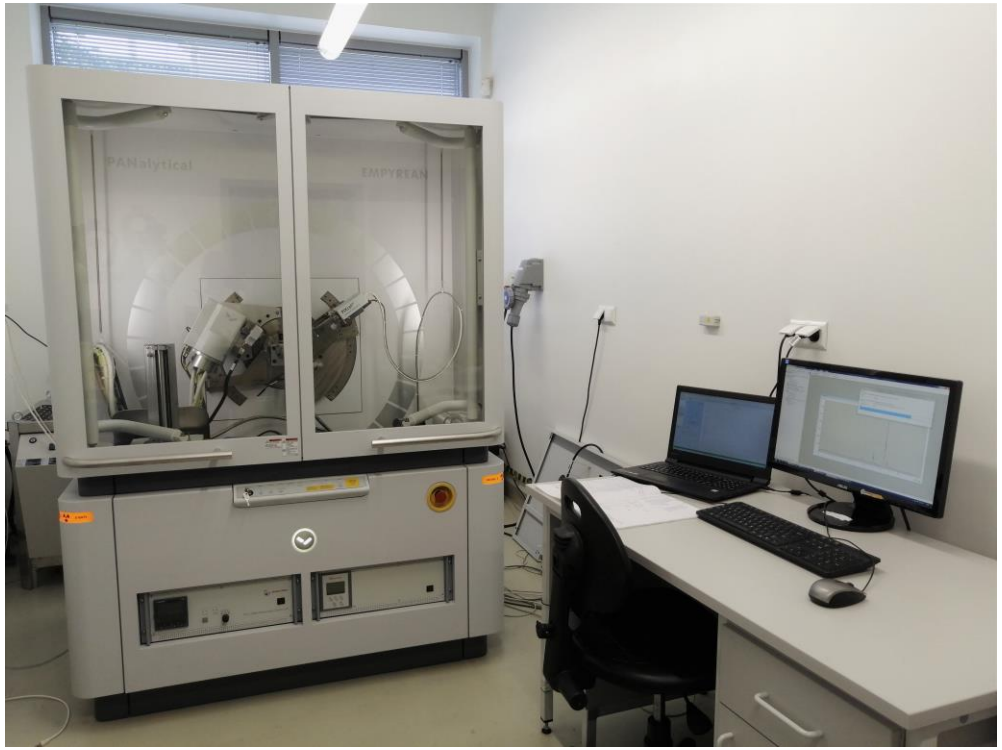
theoretical capacity
180 mAh/g

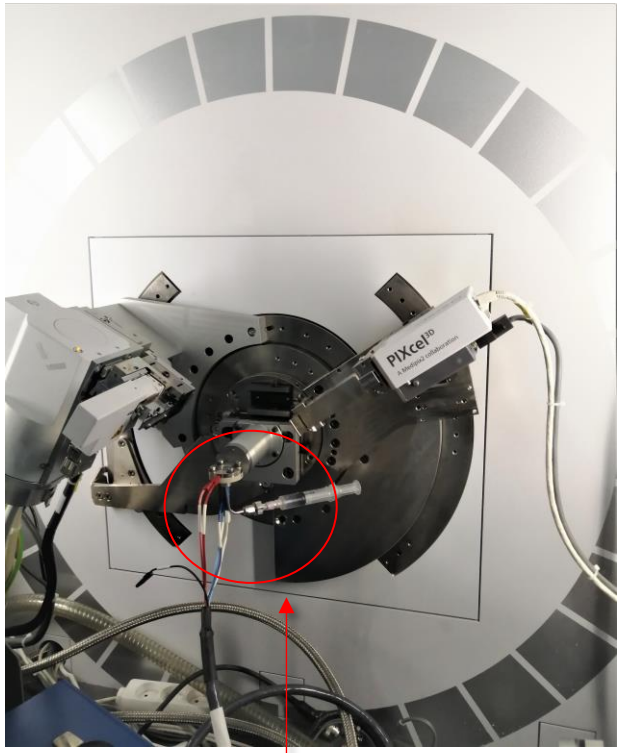
Research and Implementation Laboratory for Lithium and Sodium Batteries

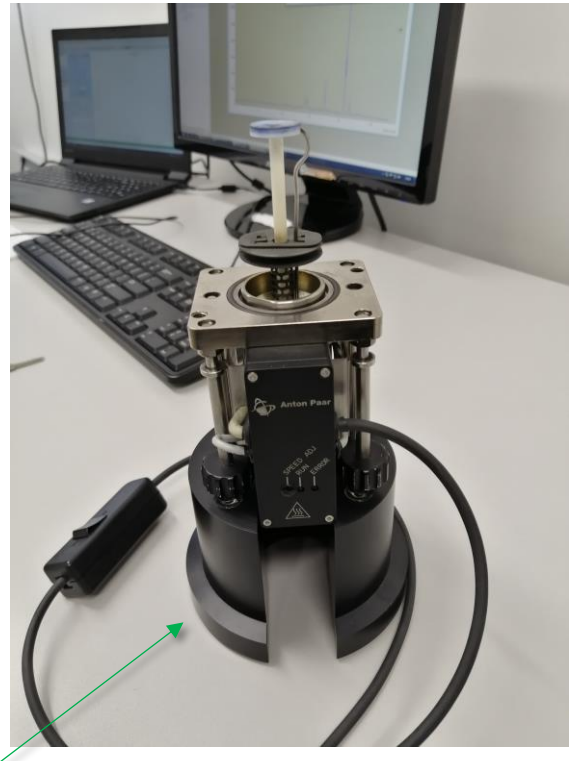
Head: Prof. J. Molenda

Center of Energy AGH-UST Kraków

X-ray difractometer







Panalytical Empyrean X-ray diffractometer

- **Dedicated in-situ cell ,allowing measurements during charge/discharge process**
- **Anton Paarhigh-temperature setup, allowing measurements in the range 300 to 1450 K**

In-situ Raman Spectrometer

DXR™3xi Raman Imaging Microscope
ThermoFisher Science

Thermo Scientific™ transfer cell for analysis of Li-ion and Na-ion battery materials

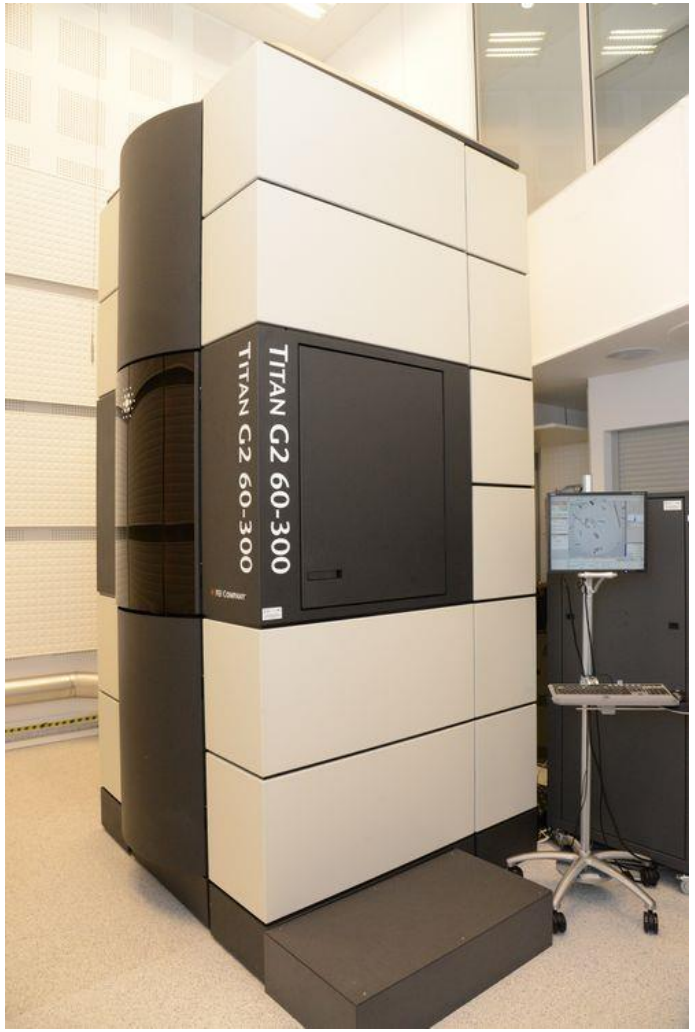
https://www.thermofisher.com/pl/en/home.html

High Resolution Transmission Electron Microscopy

HRTEM measurements in cooperation with

International Centre of Electron Microscopy for Materials Science

AGH University of Science and Technology

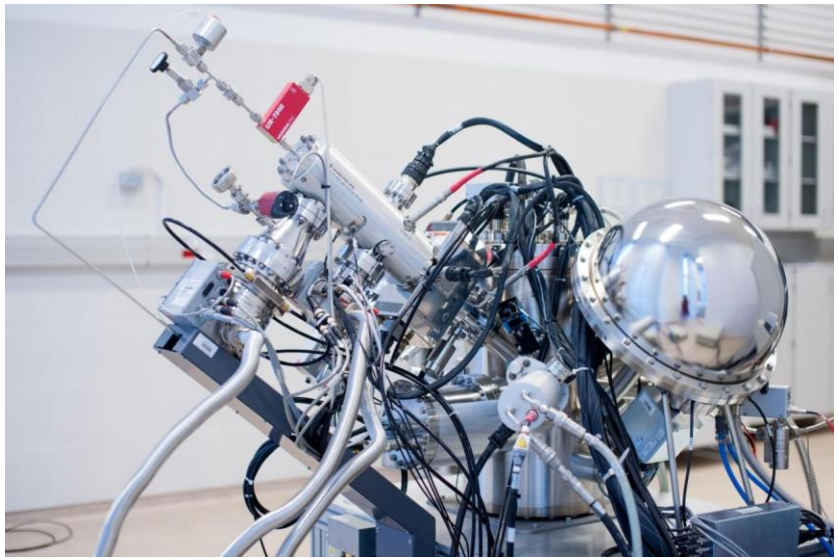


Titan Cubed G2 60-300 (FEI) - a probe Cs corrected (S)TEM for analytical high resolution microscopy (70pm) at high (300 kV) and low (60 kV) voltage (https://www.tem.agh.edu.pl/main_new/index.php/en/10-kategoria-pl-pl/21-titan-cubed-2-60-300-fei)

X-ray photoelectron spectroscopy

XPS measurements in cooperation with

Academic Centre for Materials and Nanotechnology
AGH University of Science and Technology

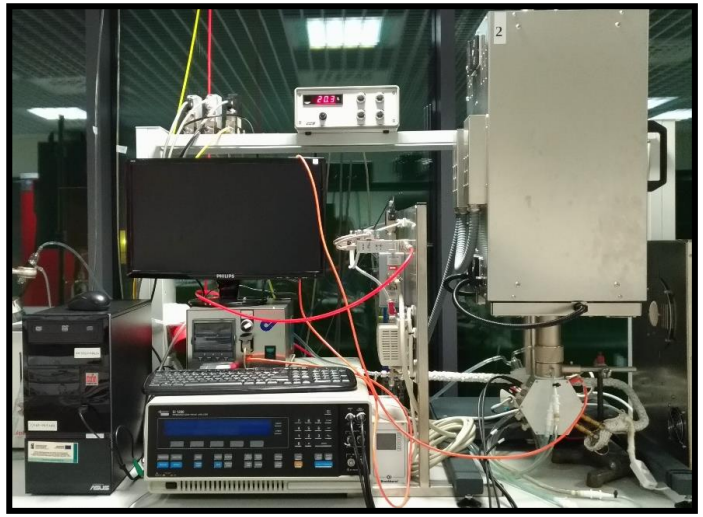


XPS/UPS PHI 5000 VersaProbeII (ULVAC-PHI, Chigasaki, Japan)
http://www.acmin.agh.edu.pl/index.php/en/

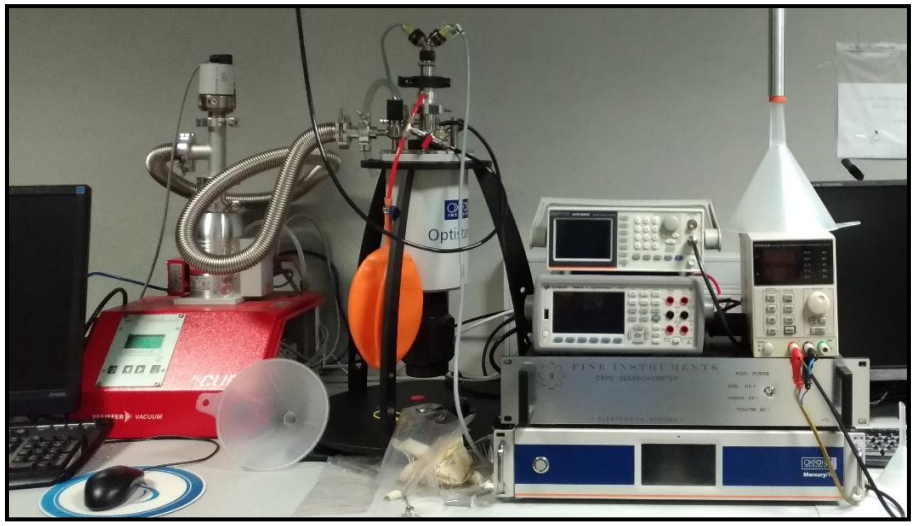
Chemistry laboratory

Physicochemical research laboratory

Physicochemical research laboratory

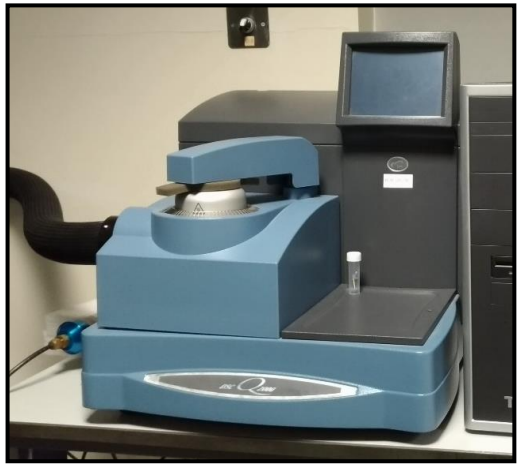


AC impedance spectroscopy measurement system with Solartron 1260 frequency response analyzer coupled with Solartron 1296 Dielectric Interface (300 to 1000 K) in controlled atmosphere



Oxford Cryostat setup, allowing measurements in the range from 20 to 300 K

Thermobalance Q5000IR TA Instruments with quadrupole mass spectrometer Pfeiffer Vacuum ThermoStar

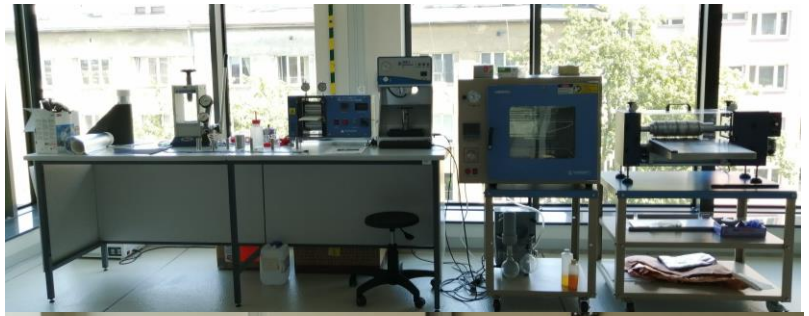


Differential Scanning Calorimeter TA Q2000 allowing measurements 80 to 600 K

Electrochemical research laboratory 1

Electrochemical research laboratory 2

Pilot-scale assembly line of Li-ion and Na-ion batteries of 18650 type



Academic Computer Centre CYFRONET AGH

http://www.cyfronet.krakow.pl/en/4421,main.html