UNIVERSITÄT LEIPZIG

Fakultät für Chemie und Mineralogie

KRAUTSCHEID Research Team

Solid state chemistry and material science

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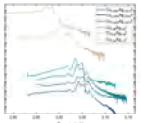
CuI as multifunctional semiconductor

CuI

- p-type direct semiconductor
- band gap 3.1 eV
- transparent
- high hole mobility



CuI single crystals

- crystal growth
- physical properties
- as substrate

CuI thin films

- Vapor phase epitaxy
- CDS
- spray pyrolysis

Tuning by doping/ alloying

- electrical properties ($CuCl_xBr_yI_{1-x-y}$; $Ag_xCu_{1-x}I$)
- optical properties
- p/n heterostructures
- magnetic properties (CuI: Co, Ni)

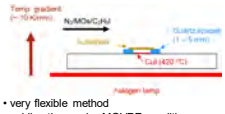
Applications:

- transparent contacts for solar cells
- highly rectifying diodes
- transparent thin-film transistors for displays

CuI single crystals

crystallization from acetonitrile solution using a precise temperature program

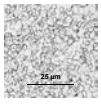
Close distance sublimation



- very flexible method
- sublimation under MOVPE conditions
- adjustment of iodine pressure in gas phase
- additions of dopants via gas phase

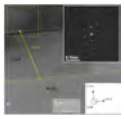
Metal organic vapor phase epitaxy (MOVPE)

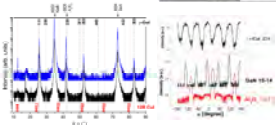
- transport of a volatile copper complex and an iodine source via gas phase
- precise total flow rate and pressure as well as partial pressures of Cu and I
  → highly reproducible conditions
- reaction in a heated reactor to form CuI and volatile by-products
- addition of doping agents via gas phase with high precision



What can I do and learn?

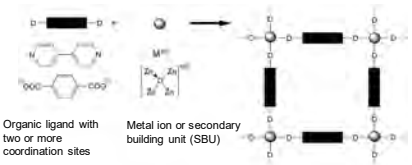
- operating MOVPE equipment and process development
- spray pyrolysis experiments
- single crystal growth and doping experiments
- layer characterization
  - ► optical and laser microscopy
  - ► electron microscopy (SEM, TEM, EDX)
  - ► X-ray diffraction
  - ► physical properties in close collaboration with the Faculty of Physics and Earth Sciences





Coordination polymers and Metal-Organic Frameworks

General concept of coordination polymers

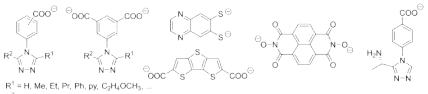


Organic ligand with two or more coordination sites

Metal ion or secondary building unit (SBU)

Coordination polymers can form one dimensional chains, two dimensional layers or three dimensional networks. The latter can have free space between the ligands. These pores make the material very promising for different applications like **gas** and **drug storage**, **catalysis**, **gas separation**, **purification**, as **sensors** etc.

MOFs in the Krautscheid group

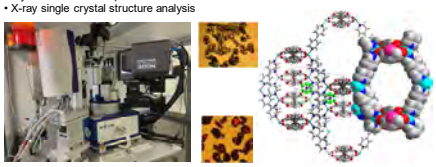


R^1 = H, Me, Et, Pr, Ph, py, $C_2H_4OCH_3$, ...
R^2 = H, Me

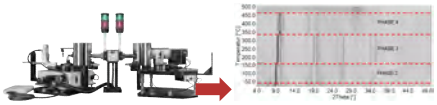
We use different ligand systems mainly based on **triazoles** coupled to aromatic systems with carboxylic groups as additional coordination sites. Dithiolene and NDI (naphthalenediimide) type ligands are used to synthesize **electrically conductive coordination polymers**.

What can I do and learn?

- ligand and MOF synthesis (diffusion methods, solvothermal, ...)
- crystallization techniques
- X-ray single crystal structure analysis

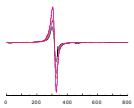


- X-ray powder diffraction (temperature dependent, different atmospheres, …)

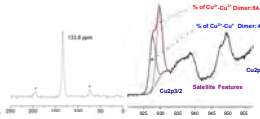


- spectroscopic characterization (IR, UV/Vis, solid state NMR, XPS, EPR, …)

EPR of a Cu MOF



solid state NMR



XPS of a Cu^+ / Cu^{2+} mixed MOF

- thermogravimetry coupled with DTA and MS
- electron microscopy (SEM, EDX)
- electrochemical investigations
- luminescence properties
- electrical conductivity
- adsorption studies
- catalysis studies

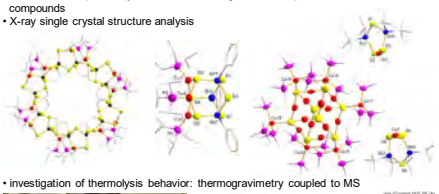
Molecular precursors for functional materials

The preparation of inorganic functional materials is normally done by solid state reactions at high temperatures in precise compliance of the reaction stoichiometry. Molecular precursors, which contain the elements of the functional material in the matching stoichiometric ratio with (mostly) organic ligands, can be thermally decomposed to obtain the functional material at moderate temperatures. We synthesize new molecular complexes as potential precursors and analyze their thermal behavior. That covers semiconductors for photovoltaic application like $Cu(Ga,In)(S,Se,Te)_2$, Cu_2SnS_3 and $(Ag,Cu)_2ZnSn(S,Se)_4$ as well as magnetic materials like $GdFeO_3$. From molecular precursors also the direct synthesis of nanoparticles is possible.

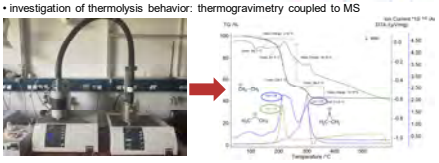
molecular precursor containing Gd, Fe and cyclohexanolate | thermolysis setup | nanoparticles of $GdFeO_3$

What can I do and learn?

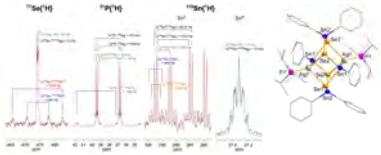
- Schlenk technique for synthesis and handling air and temperature sensitive compounds
- X-ray single crystal structure analysis



- investigation of thermolysis behavior: thermogravimetry coupled to MS



- spectroscopic characterization (heteronuclear NMR, EPR, IR, UV/Vis …)



- X-ray powder diffraction (temperature dependent)
- electron microscopy (SEM, TEM, EDX)
- magnetic properties
- etc.

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