

MATERIAL-WISSENSCHAFT

TECHNISCHE UNIVERSITÄT DARMSTADT

FORSCHUNG VERKNÜPFEN KOMPETENZEN BÜNDELN

Herzlich Willkommen zum Industrietag Materialwissenschaft 2023

Katrin Binner

14.11.2023

MATERIAL-
WISSENSCHAFT

TECHNISCHE
UNIVERSITÄT
DARMSTADT

PROF. DR.-ING. MATTHIAS OECHSNER

Vizepräsident für Forschung

14.11.2023



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HERZLICH WILLKOMMEN

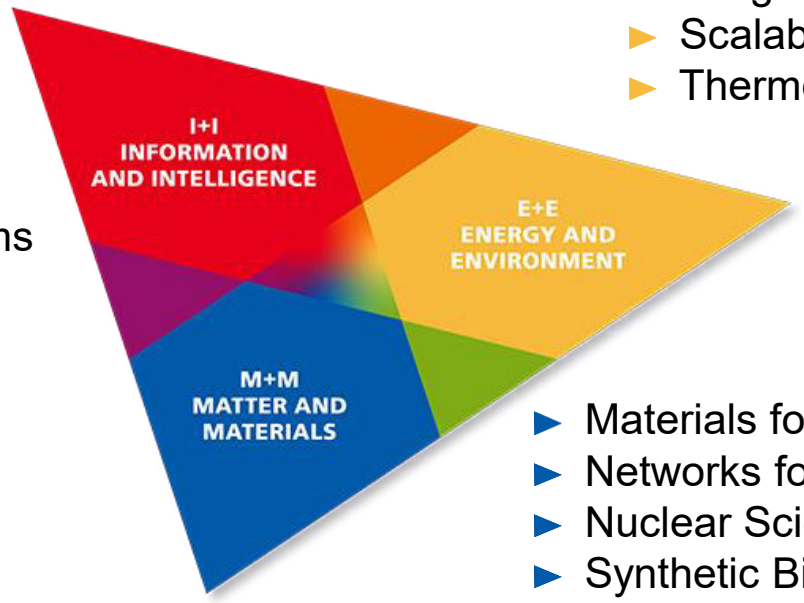
TU DARMSTADT – VERANTWORTUNG FÜR TRANSFORMATION

TECHNISCHE UNIVERSITÄT DARMSTADT

FORSCHUNGSFELDER & PROFILTHEMEN

- Carbon-Neutral Circles
- Computational Engineering
- Integrated Energy Systems
- Scalable Clean Water Cycles
- Thermo-Fluids and Interfacial Phenomena

- Artificial Intelligence
- Cognitive Science
- Complex Interconnected Systems
- Cybersecurity and Privacy

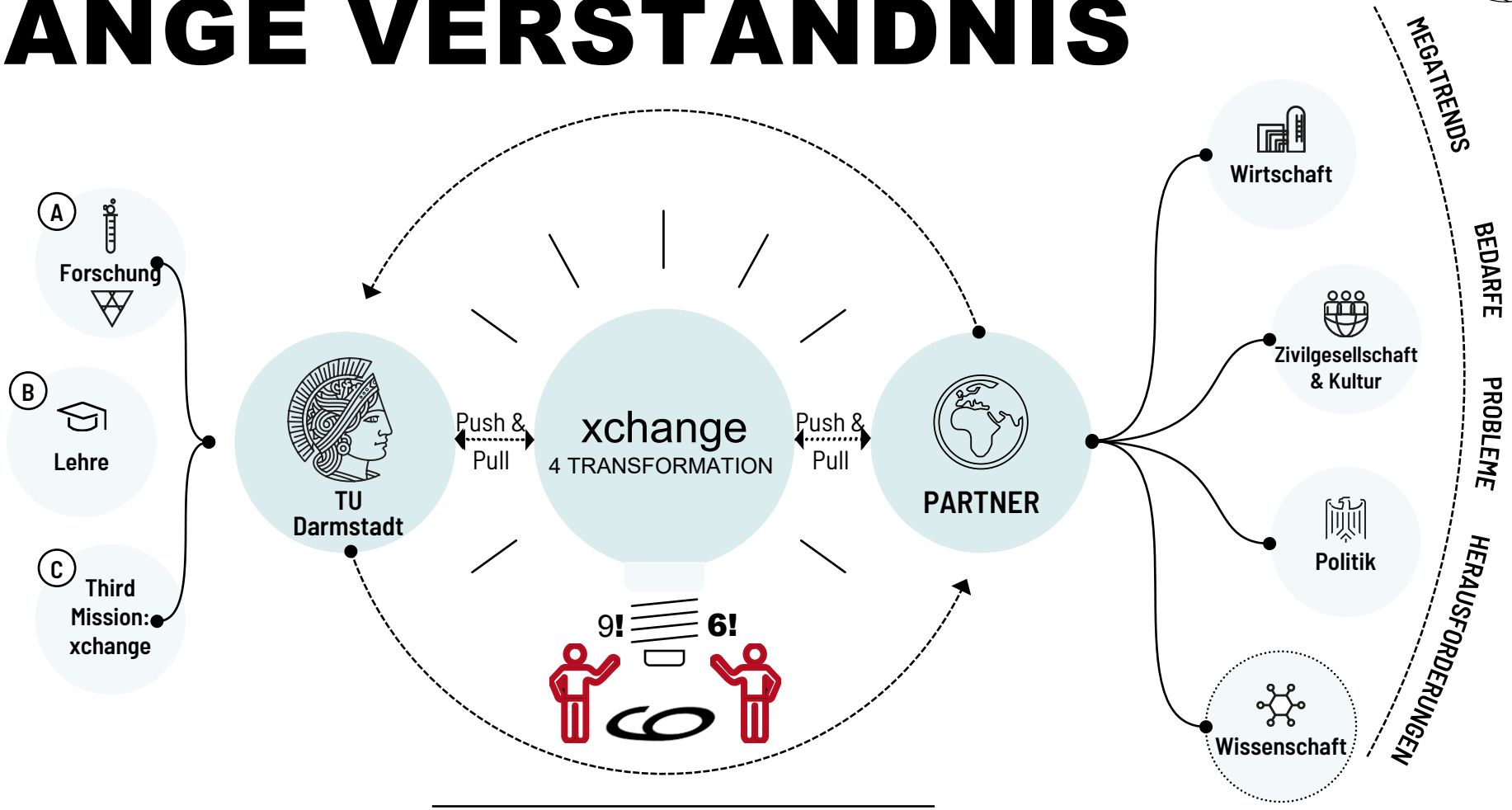


- Materials for Circularity
- Networks for Industry 4.0
- Nuclear Science
- Synthetic Biology

Blick auf die gesamte Wertschöpfung: Von der Grundlage bis in die Anwendung

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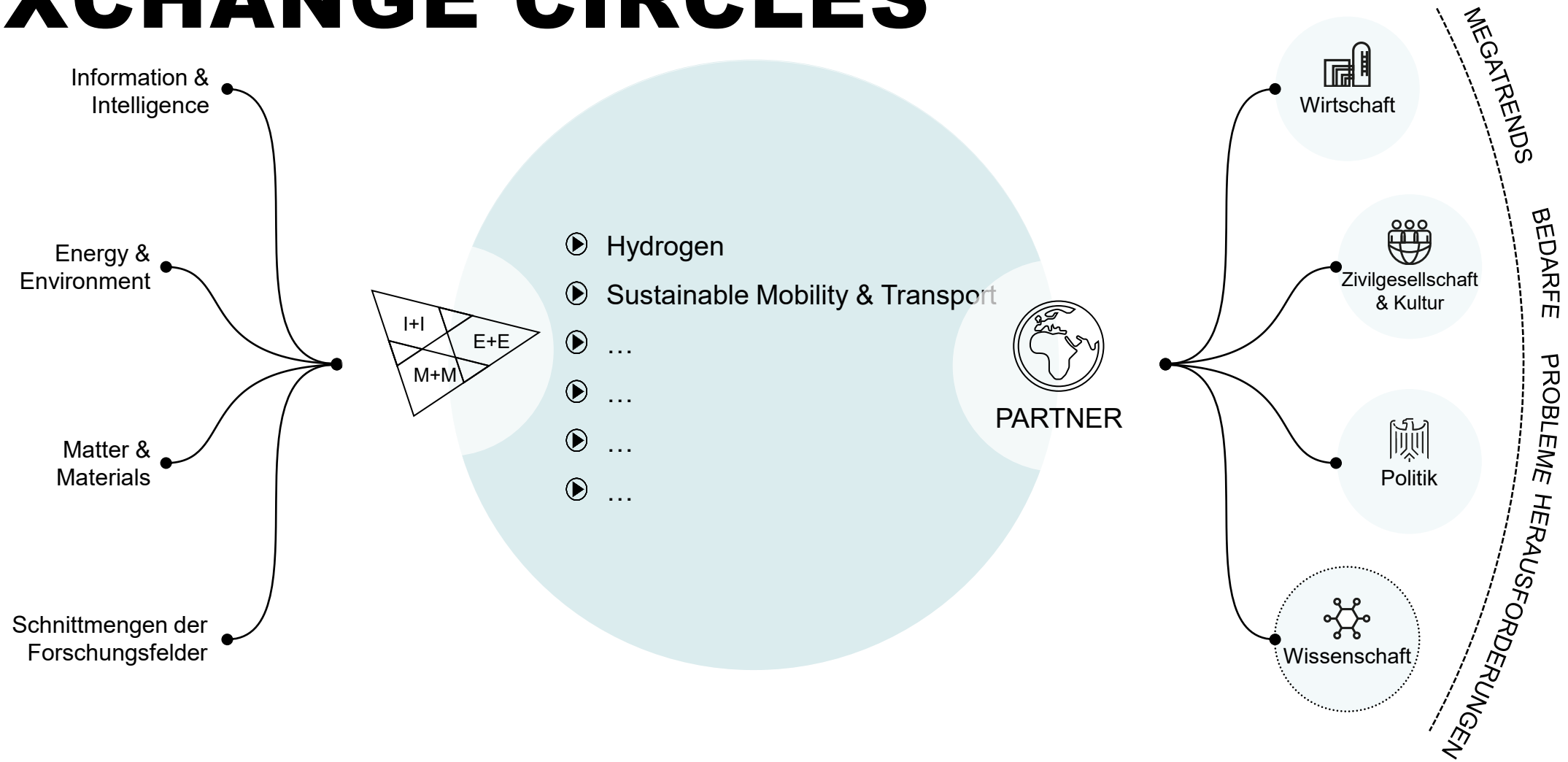
XCHANGE VERSTÄNDNIS



Austausch & Übersetzung von Wissen, Methoden und Technologien, um Transformation zu gestalten

TECHNISCHE UNIVERSITÄT DARMSTADT

XCHANGE CIRCLES



TECHNISCHE UNIVERSITÄT DARMSTADT



PROF. DR.-ING.

MATTHIAS OECHSNER

Vizepräsident für Forschung
Technische Universität Darmstadt

vp-forschung@tu-darmstadt.de

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TECHNISCHE
UNIVERSITÄT
DARMSTADT

PROF. DR. WOLFGANG DONNER

Dekan Fachbereich 11 – Material- und Geowissenschaften

14.11.2023



INSTITUT FÜR MATERIALWISSENSCHAFT

© Thomas Ott

TECHNISCHE UNIVERSITÄT DARMSTADT

ECKDATEN

18 Fachgebiete (inkl. 3 gemeinsam koordinierter Berufungen mit GSI und KIT und 1 Kooperationsprofessur)

58 Beschäftigte

200 Promovierende und PostDocs

500 Studierende



FORSCHUNG

ENERGIE – SUBSTITUTION – ZIRKULARITÄT

2 Sonderforschungsbereiche

Dichtes nationales und internationales Netzwerk

SFB/TRR 270 HoMMage

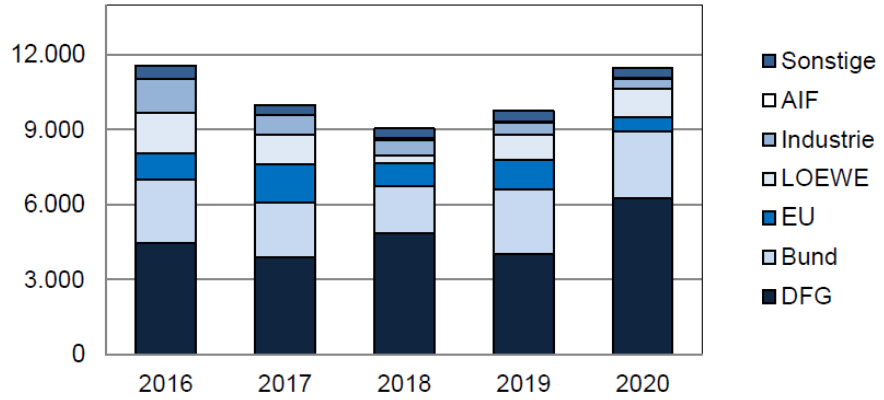
FLAIR

Fraunhofer IWKS

KIT

GSI

Drittmittel



LEHRE

2 STUDIENGÄNGE

B.Sc. Materialwissenschaft

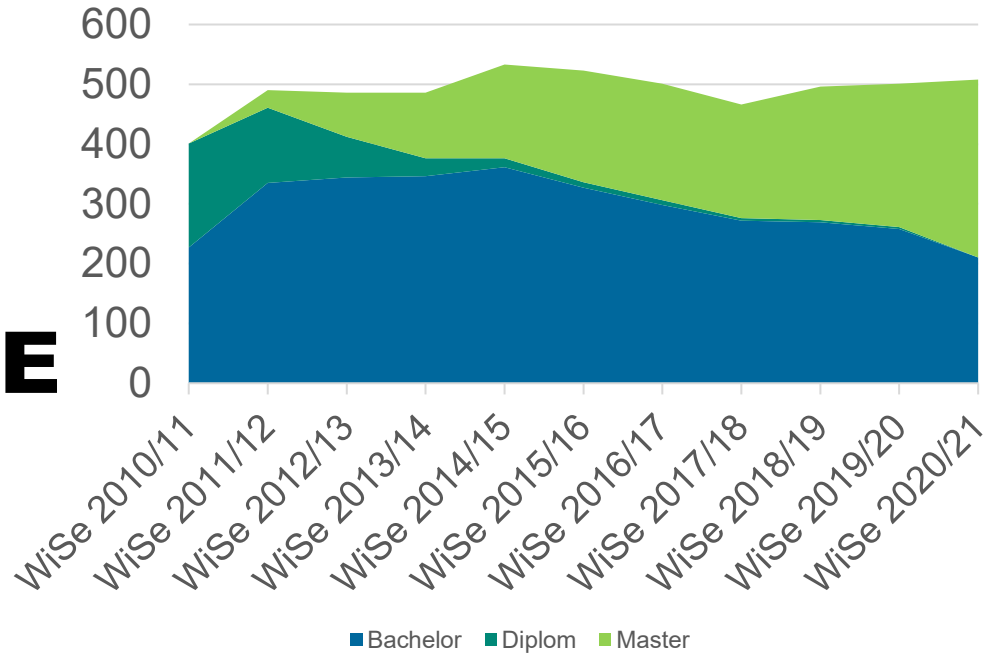
M.Sc. Materials Science

3 EU MASTERPROGRAMME

Advanced Materials: Innovative Recycling

Functionalized Advanced Materials and Engineering

Advanced Materials for Innovation and Sustainability



AMIR master

Co-funded by the European Union

FAME AIS MASTER

AMIS MASTER

Advanced Materials for Innovation and Sustainability

TECHNISCHE UNIVERSITÄT DARMSTADT

KOMPETENZZENTRUM MATERIALCHARAKTERISIERUNG

DIENSTLEISTUNGSANGEBOT

Beteiligte sind die Fachgebiete der Materialwissenschaft,

Zusammenarbeit mit der Materialprüfungsanstalt (MPA)

Zur Zeit mehr als 600 Kunden aus der Industrie und Forschungsinstituten



Dr. Joachim Brötz

Kontakt
joachim.broetz@tu-...
+49 6151 16-21030

“UMFASSENDE MATERIALCHARAKTERISIERUNG AUS EINER HAND“

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DR. PHILIPP WALTER

Geschäftsführer Materials Valley e.V.

14.11.2023

materials valley

Profilierung der Region RheinMain als High Tech-Standort für Materialforschung und Werkstofftechnologie

- **Materials Valley e.V.** in 2002 gegründet

- **Mitglieder**
  Industrieunternehmen, Hochschulen, Forschungsinstitute, Instutionen der Länder zur Förderung von Technologie und Wirtschaft

- **Ziele**
  - Ausbau von Wissensnetzen zu einem Forschungsverbundnetz
  - Gestaltung von attraktiven wissenschaftlichen und sozialen Bedingungen im Materials Valley für hoch-qualifizierte Arbeitskräfte und Studenten
  - Kommunikationsplattform für Wirschaft und Wissenschaft
  - Organisation von Vortragsreihen

Materials Valley und Technologieland Hessen haben folgende Reihen veranstaltet







Links

www.materials-valley.de

https://www.technologieland-hessen.de/materials-for-the-Egd

https://redaktion.hessen-agentur.de/publication/2022/3782_EuropeanGreenDeal_Web.pdf

https://www.technologieland-hessen.de/RePowerEU

redaktion.hessen-agentur.de/publication/2023/4099_MaterialstoRePowerEU.pdf

→ Nächste Veranstaltungsreihe in 2024 über “Critical Raw Materials”

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HERAEUS PRECIOUS METALS

Standnummer 03



INTRODUCTION TO HERAEUS

2023

THE HERAEUS GROUP – A FAMILY-OWNED TECHNOLOGY COMPANY

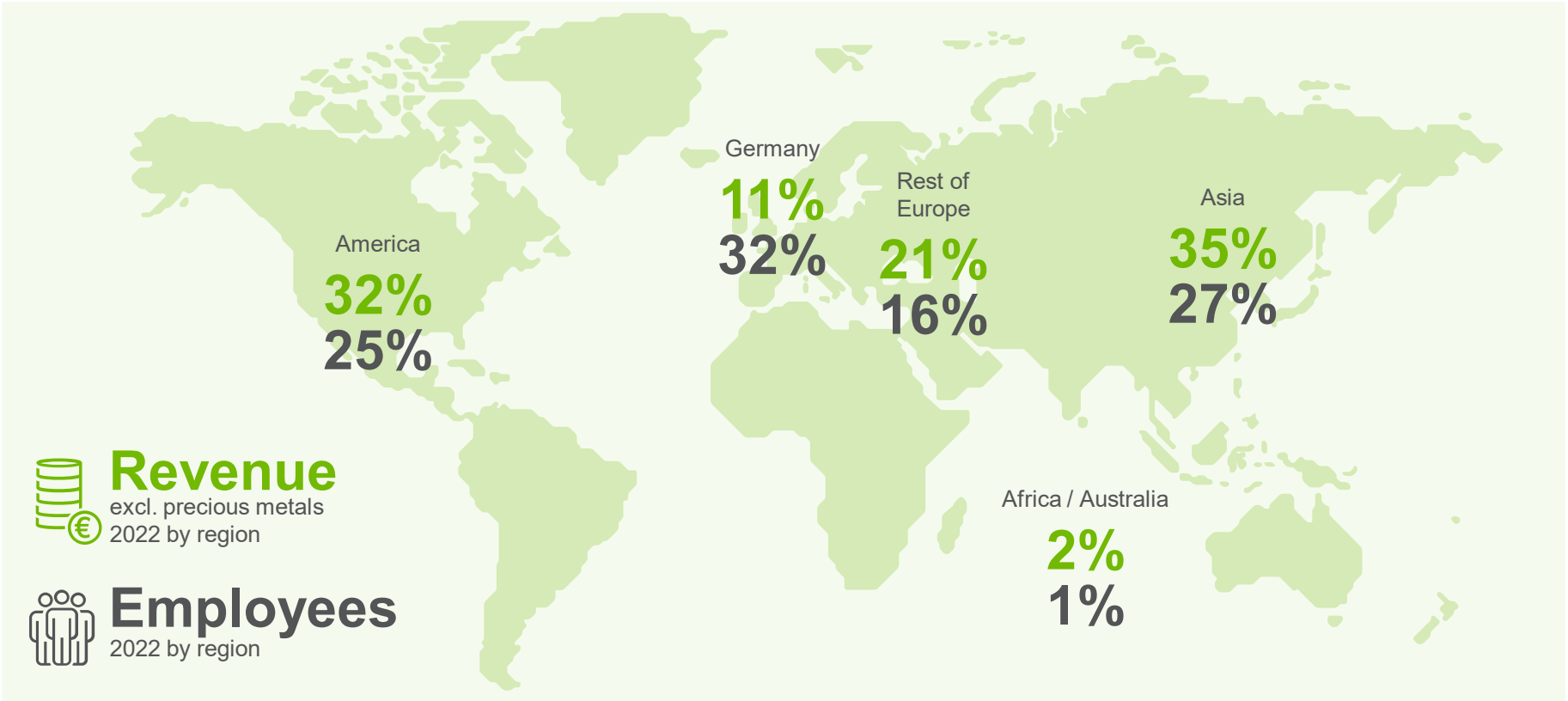
Total Revenue in 2022

29.1 bn. €
(30.6 bn. US$)

US$ calculated with 2022 average exchange rate (1€ = 1.0530 US$)

More than **100** sites in **40** countries

market-oriented distribution in **20 Operating Companies**



Revenue
excl. precious metals
2022 by region

Employees
2022 by region

5.4%
R & D Expenditures
based on revenues excl. Precious Metals

APPROX. **17,200**
employees worldwide
incl. staff leasing

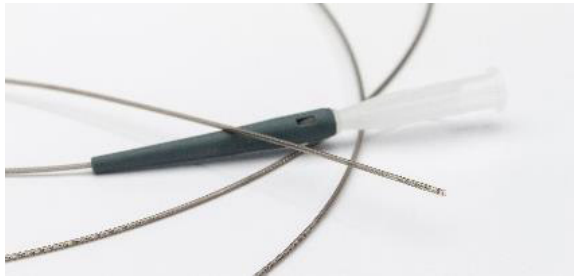
TOP 10
family-owned companies
in Germany

A DIVERSE PRODUCT PORTFOLIO MEETS CUSTOMER NEEDS



Bone cement

with antibiotics to prevent infection risks during fixation of joint replacements



Implants and catheters

for minimally invasive treatments and neurostimulation



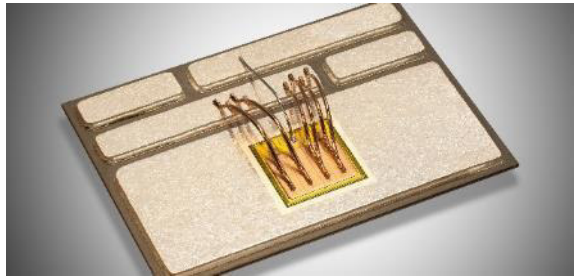
Fused silica

for the semiconductor and telecommunications industry



Silver pastes

for higher efficiencies of solar cells



Metal-ceramic substrates

for power electronics



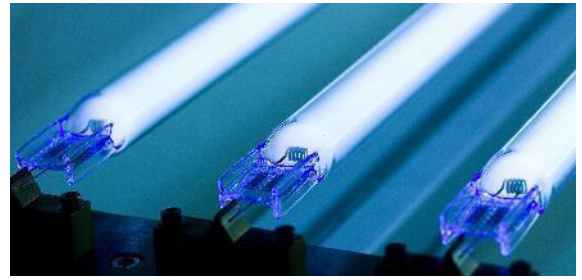
Precious metals

trading, recycling, industrial processing



Sensors

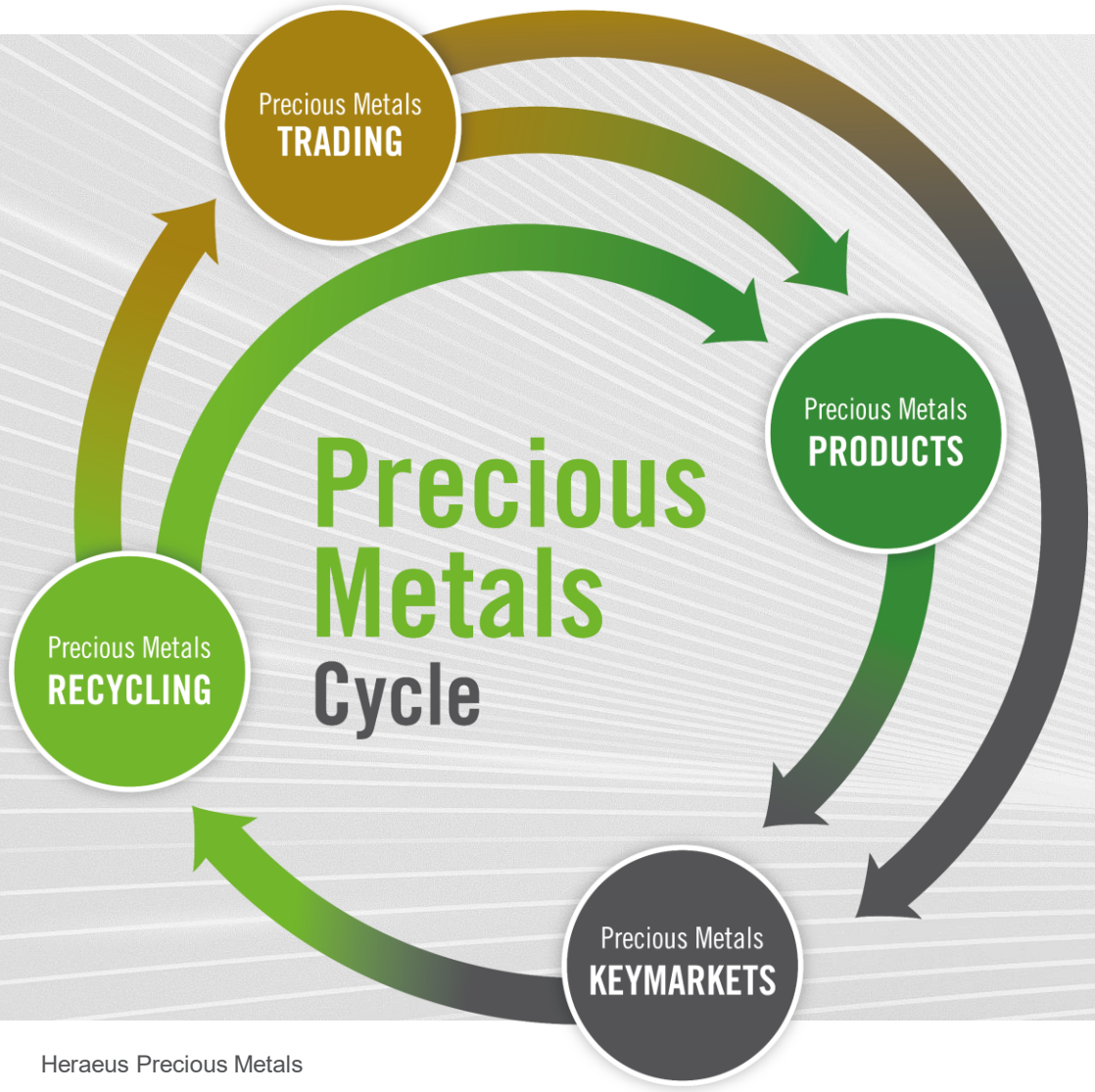
for measurements in molten metals



Special light sources

from ultraviolet to infrared for a wide range of applications

HERAEUS REFINES ALL 8 PRECIOUS METALS



	Total annual production 2022 global Primary and secondary sources	Recycling-share 2022 global
79 Au Gold 196.9665	4.800 t	30 %
47 Ag Silver 107.8682	32.200 t	25 %
78 Pt Platinum 195.084	225 t	30 %
46 Pd Palladium 106.42	280 t	40 %
45 Rh Rhodium 102.9055	32 t	45 %
44 Ru Ruthenium 101.07		
77 Ir Iridium 192.217		
76 Os Osmium 190.23		

Source: Metals Focus | Heraeus
Total figures worldwide, all recycling and refining companies

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TU DARMSTADT - OBERFLÄCHENFORSCHUNG

Standnummer 04

14.11.2023

Das Fachgebiet Oberflächenforschung

Industrietag Materialwissenschaft 2023

Prof. Dr. rer. nat. Jan Philipp Hofmann

TECHNISCHE UNIVERSITÄT DARMSTADT

Surface Science

Kontaktdetails:
Prof. Dr. Jan Philipp Hofmann
Fachgebiet Oberflächenforschung (Surface Science Lab)
FB Material- und Geowissenschaften
TU Darmstadt
Gebäude L1|08, Raum 227
Otto-Berndt-Straße 3
64287 Darmstadt

E-mail: hofmann@surface.tu-darmstadt.de

tel.: +49-6151-16-20769 @SurfSciLab_DA

SCAN ME

www.mawi.tu-darmstadt.de/of

Das Fachgebiet Oberflächenforschung



Zurzeit:

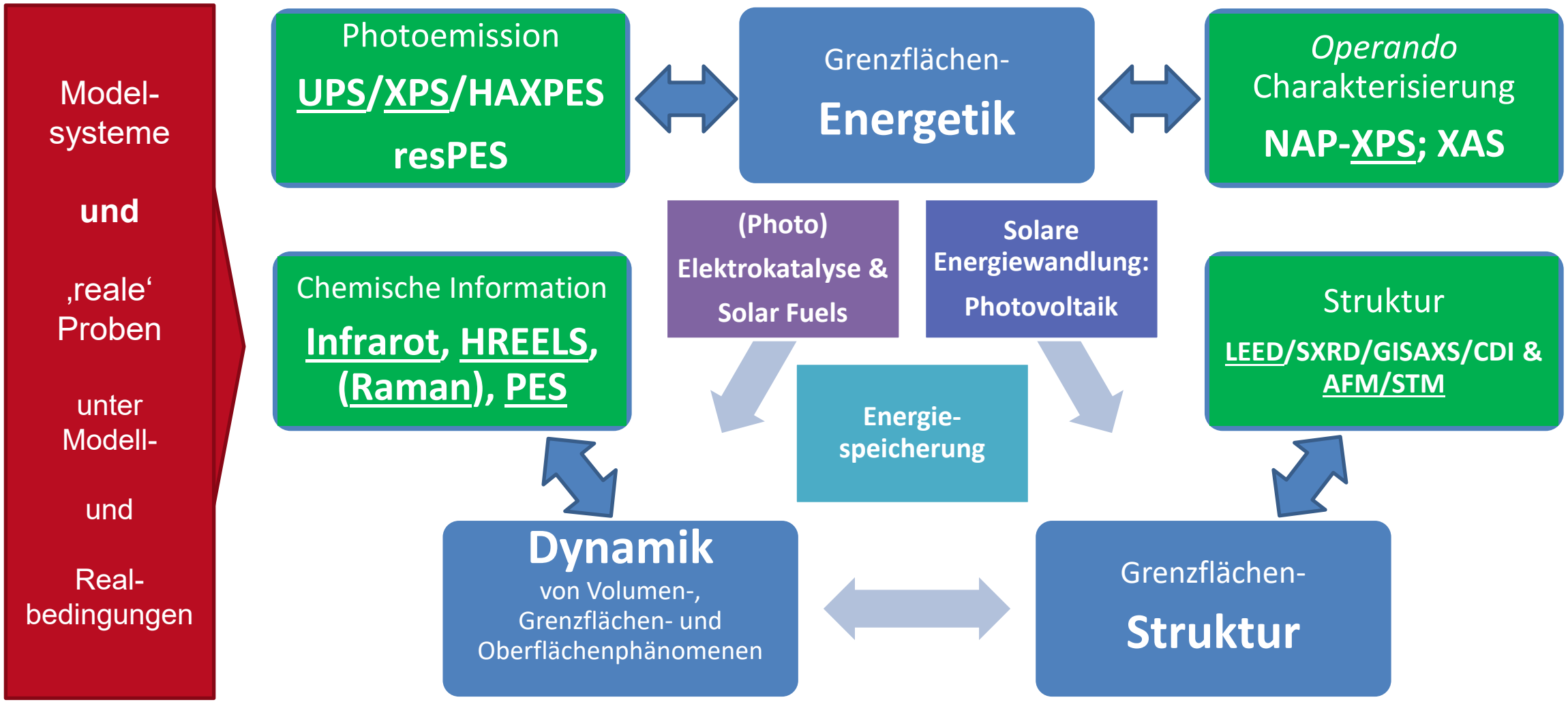
1 Prof.
2 Postdocs
12 Doktorand:innen
1 Technikerin
1 Ingenieur
1 Sekretärin



Die **Mission des Fachgebiets Oberflächenforschung** ist es, das Grundlagenverständnis der chemischen und physikalischen Prozesse, der Energetik und der Dynamik von Oberflächen und Grenzflächen in Materialien und Bauelementen für die Wandlung und Speicherung erneuerbarer Energien zu vergrößern und anzuwenden.

Der Surface Science Ansatz

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Unsere DAISYs

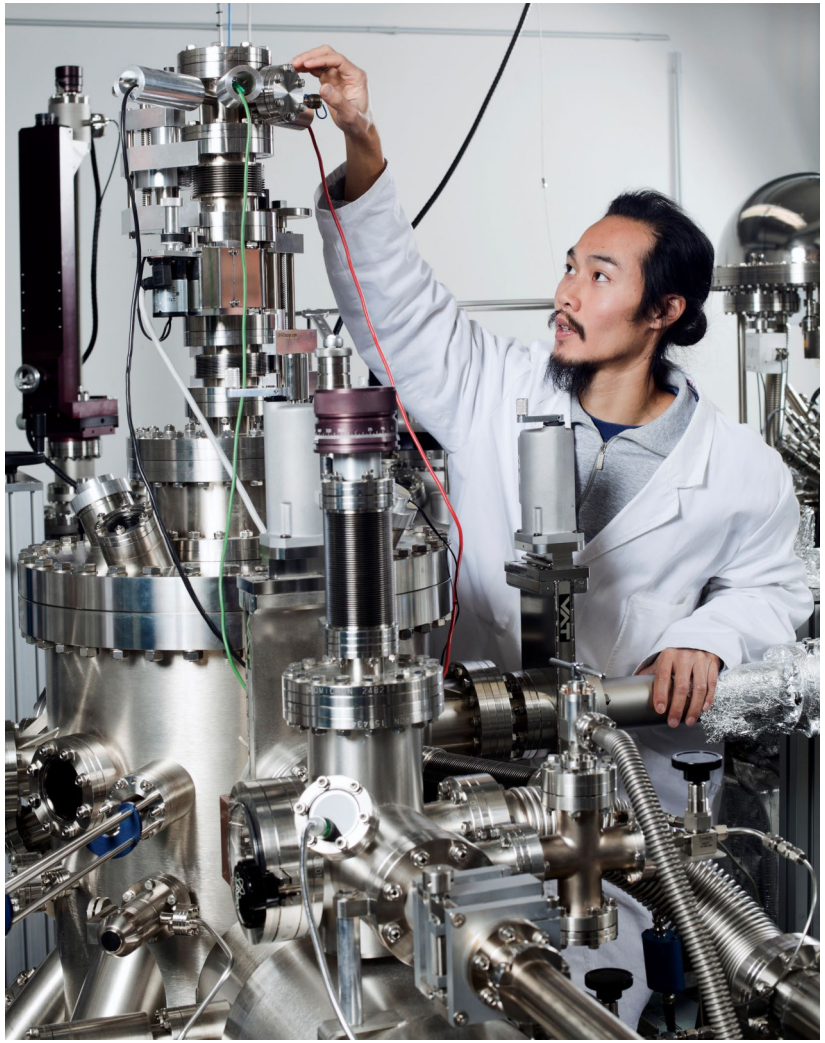
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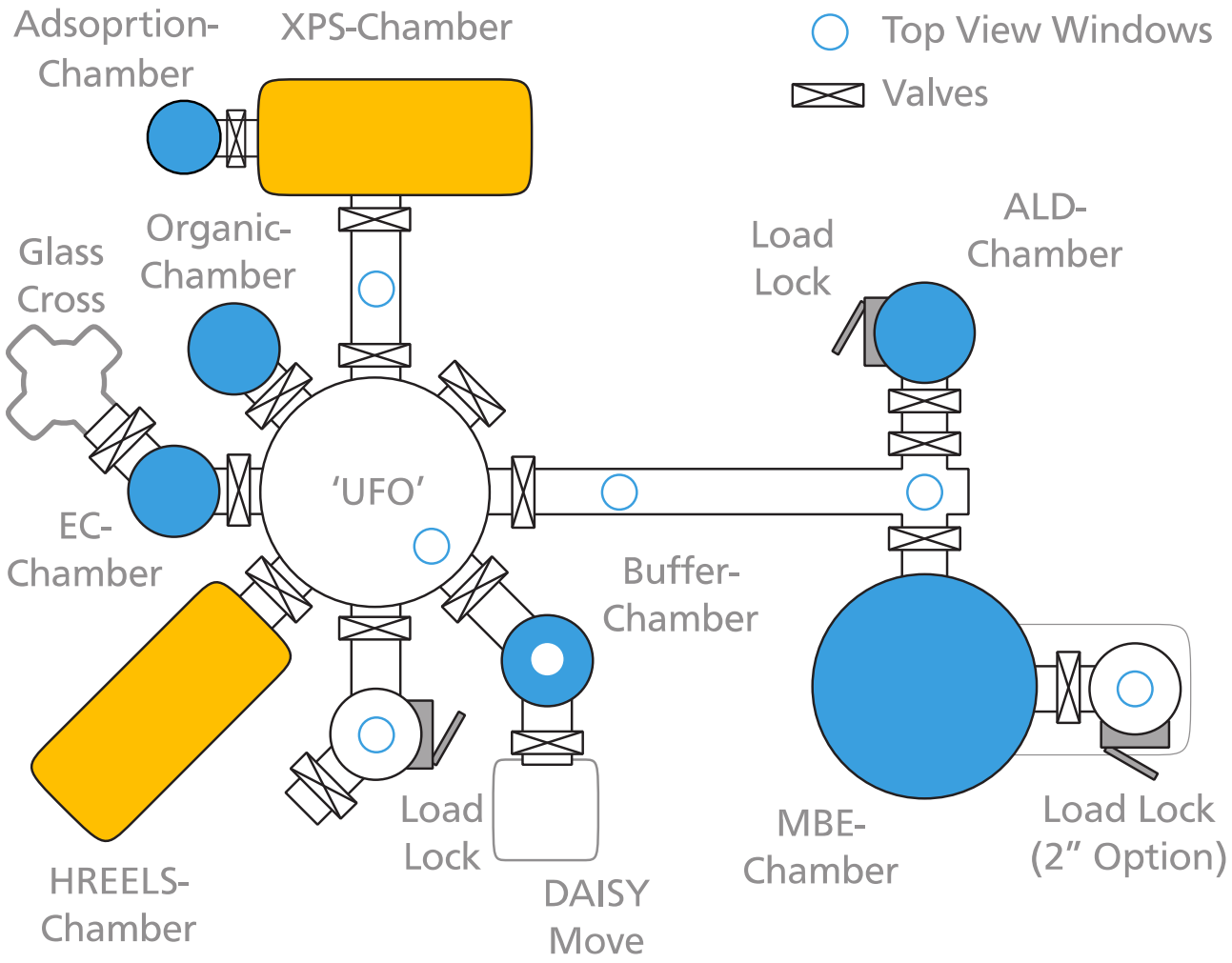
- a.k.a. Darmstädter Integrierte Systeme
- Integration von Dünnschichtherstellung und Charakterisierung in einem Vakuumsystem
- **DAISY-FUN:** DAISY für fundamentale Untersuchungen in der Oberflächenphysik/-chemie mit Fokus Elektrokatalyse
- **DAISY-BAT:** DAISY für Batterieforschung (Li/Na Ionenbatterien)
- **DAISY-SOL:** DAISY für Solarzellenforschung
- **SOLIAS:** Solid-Liquid Interface Analysis System am BESSY II Synchrotron in Berlin



© Disney

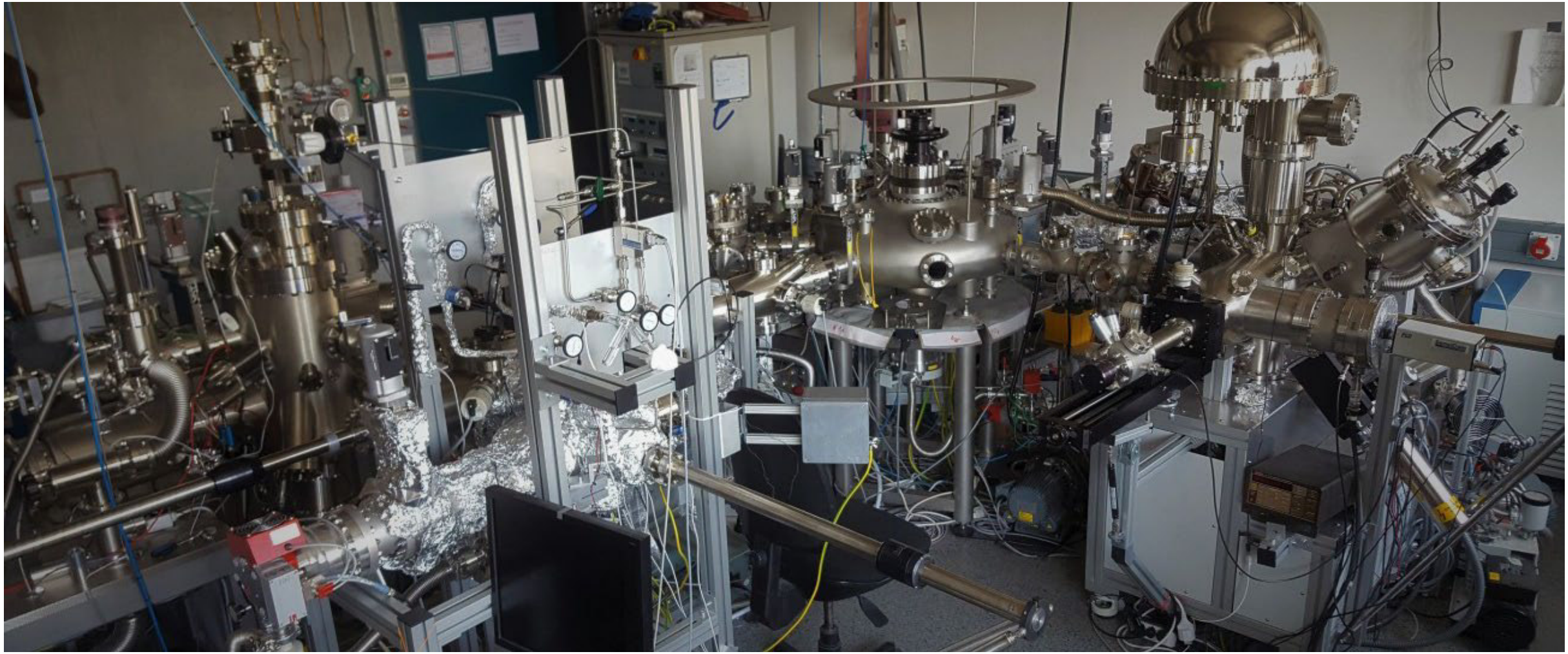
DAISY-FUN




Adsoprtion-
Chamber
XPS-Chamber
Top View Windows
Valves
Glass
Cross
Organic-
Chamber
Load
Lock
ALD-
Chamber
'UFO'
EC-
Chamber
Buffer-
Chamber
HREELS-
Chamber
Load
Lock
DAISY
Move
MBE-
Chamber
Load Lock
(2" Option)

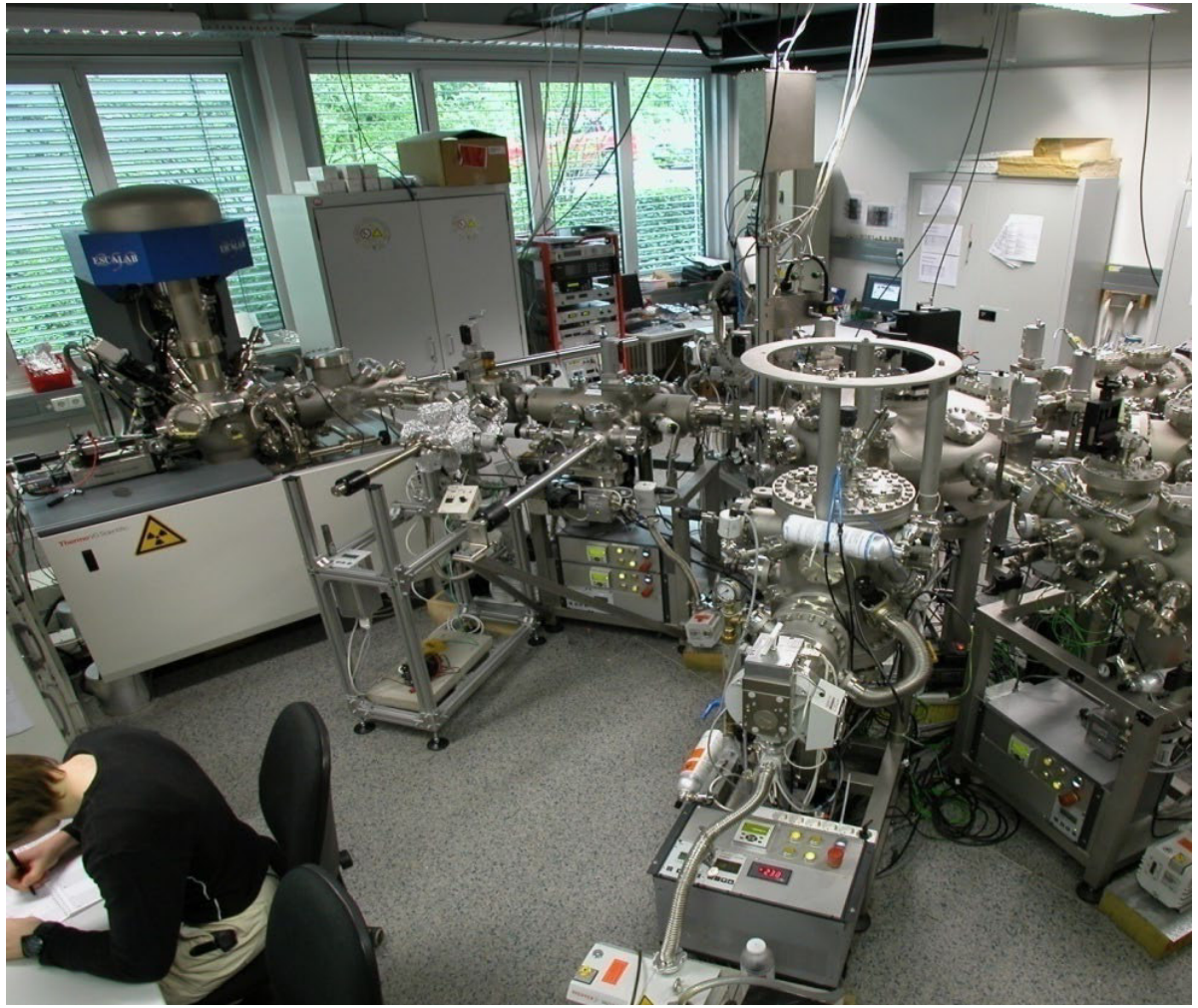
DAISY-FUN

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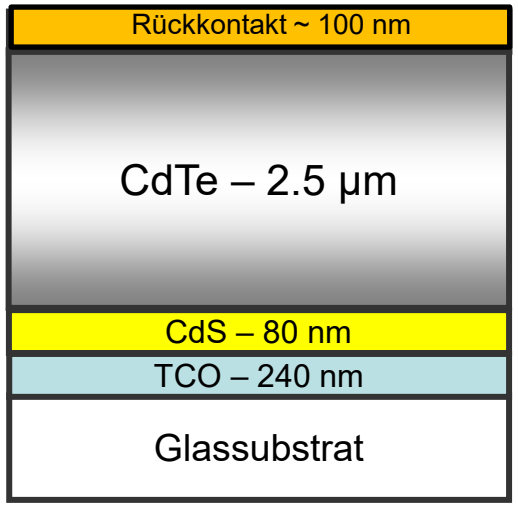


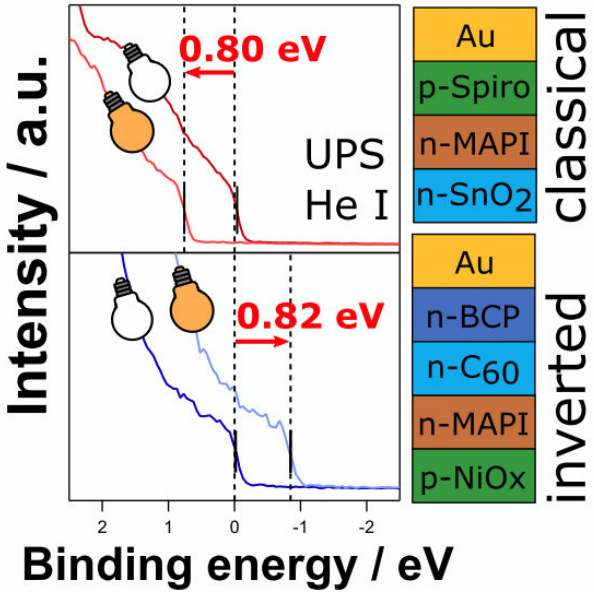
DAISY-SOL

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Hier können komplette Solarzellen im Vakuum hergestellt und jeder Einzelschritt charakterisert werden!





Vielen Dank für Ihre Aufmerksamkeit!

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DARMSTADT

TU DARMSTADT – ADDITIVE MANUFACTURING CENTRE

Standnummer 05

14.11.2023

Additive Manufacturing Center – AMC
Technologie- und Wissenstransferzentrum

Darmstadt | 04.10.2023

TECHNISCHE UNIVERSITÄT DARMSTADT

ADDITIVE MANUFACTURING CENTER

Investition in Ihre Zukunft

Kofinanzierung durch die
Europäische Union aus dem
Europäischen Fond für regionale Entwicklung

HESSEN Hessisches Ministerium für Wirtschaft, Energie, Verkehr und Landesentwicklung



Quelle: Nickl Architekten, München

AMC als Co-Working Space zwischen Industrie und Wissenschaft (ab Januar 2023)

ADDITIVE MANUFACTURING CENTER

TECHNISCHE UNIVERSITÄT DARMSTADT

Das AMC als öffentliches Technikum bietet:

- Arbeitsräume für interdisziplinäre Zusammenarbeit
- Projektarbeitsräume für kooperativen Technologie-Transfer
- Abbildung der kompletten Prozesskette „vom Rohstoff bis zum Recycling“

Hierfür stehen bereit:

Technikum

- 80 m² Pulverherstellung
- 180 m² AM-Labor
- 120 m² Fabrikhalle
- 180 m² Analytik

Büro und Co-Working-Spaces

- CAD-Lab für die digitale Prozesskette
- Schulungs- und Seminarräume
- Agile Projektbüros
- MakerLab zur Überführung digitaler Daten in physische Demonstratoren

PTW TU DARMSTADT

MPA IfW Darmstadt

RESOURCES MATERIALS

PhM

pmd produktentwicklung maschinenelemente

SAM

LSM Lightweight Engineering and Structural Mechanics

Datenverarbeitung in der Konstruktion

FUNKTIONALE MATERIALIEN

idd

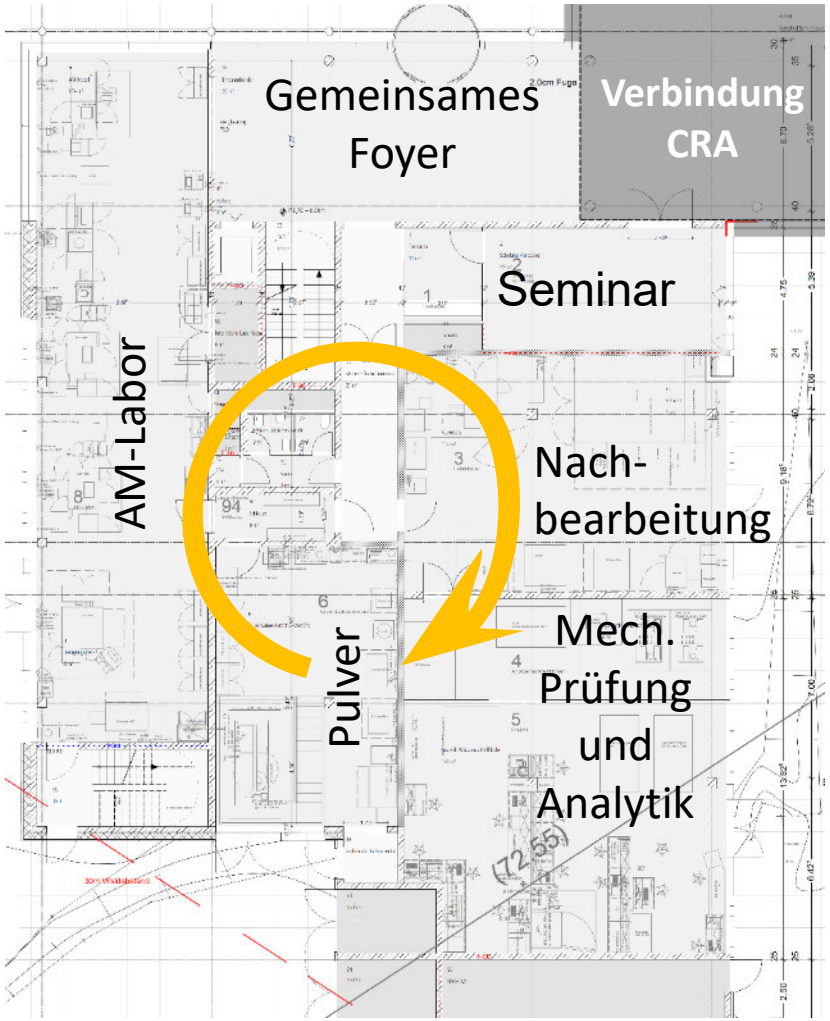
ISM+D Institute of Structural Mechanics and Design Institut für Statik und Konstruktion

CPS Cyber-Physical Simulation TU Darmstadt

Neubau des Additive Manufacturing Center
GRUNDRISS ERDGESCHOSS / TECHNIKUMSEBENE

ADDITIVE MANUFACTURING CENTER

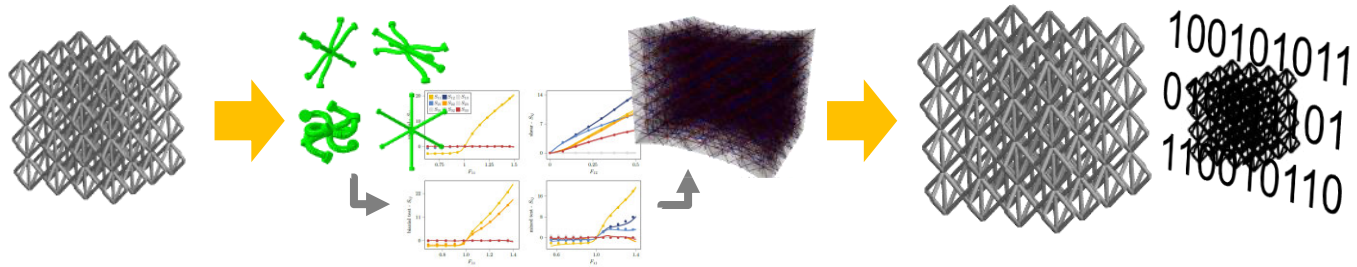
TECHNISCHE UNIVERSITÄT DARMSTADT



- Technikumsebene zur Abbildung der kompletten Prozesskette

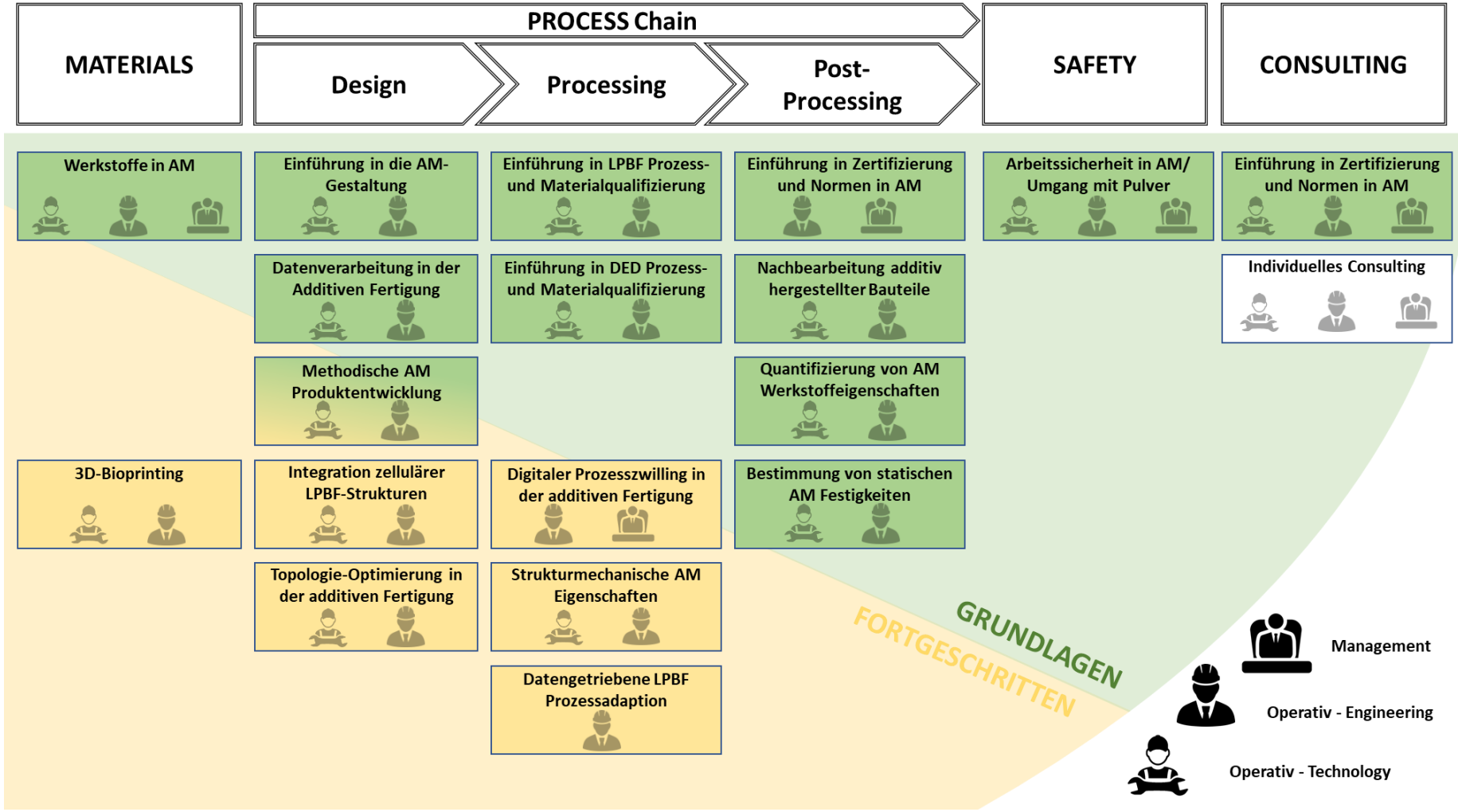


- Digitale Abbildung entlang der Wertschöpfungskette



- Seminarraum zur Veranstaltung von Schulungen und Workshops

Schulungskatalog



- „One-Stop-Shop“ für Schulungen entlang der kompletten Prozesskette
- Individuelle Pakete zusammenstellbar
- Kombination mit „Hands-On“-Workshops im Technikum

www.tu-darmstadt.de\amc

ADDITIVE MANUFACTURING CENTER

TECHNISCHE UNIVERSITÄT DARMSTADT

- Expertise in the fields of **Additive Manufacturing** and **digital transformation**
- Industry meets Science
- Wide range of **workshops**, **trainings** and **education**
- Focussing on **SME**



Start on January 1st, 2023
Join us!

- **600 qm Lab for AM, powder production, analytics and post processing**
- **Digital Lab and maker lab allow practical experience**
- **Seminar rooms and co-working spaces**

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TU DARMSTADT – FUNKTIONALE MATERIALIEN

Standnummer 06

14.11.2023

FUNKTIONALE MATERIALIEN

TECHNISCHE UNIVERSITÄT DARMSTADT

FUNCTIONAL MATERIALS

Prof. Oliver Gutfleisch

MAX-PLANCK-INSTITUT FÜR EISENFORSCHUNG GmbH

Fraunhofer IWKS

MAGNOTHERM®

DFG Deutsche Forschungsgemeinschaft

erc

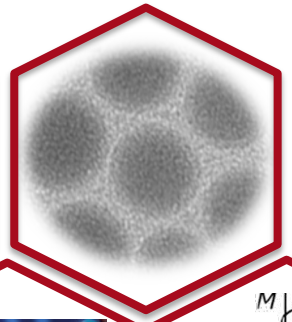
FM - RESEARCH TOPICS

TECHNISCHE UNIVERSITÄT DARMSTADT

Magnetic cooling
Hydrogen liquefaction



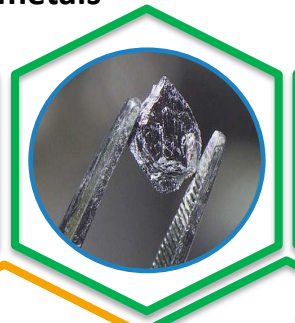
Magnetic nanoparticles for biomedicine



Advanced measurement systems



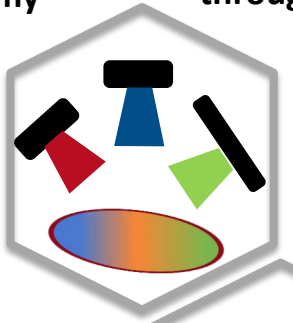
Criticality of technology metals



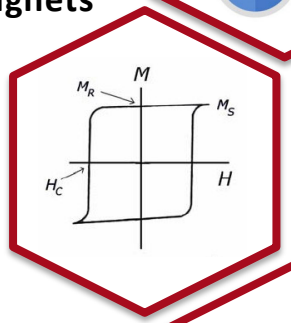
Circular economy

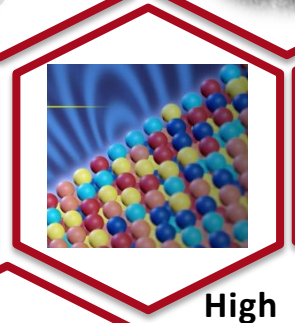


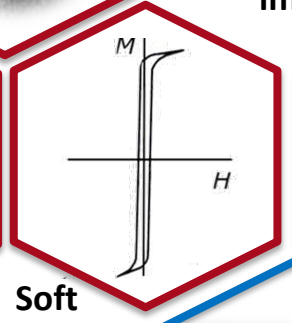
High throughput



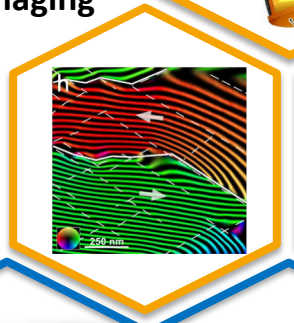
Hard magnets

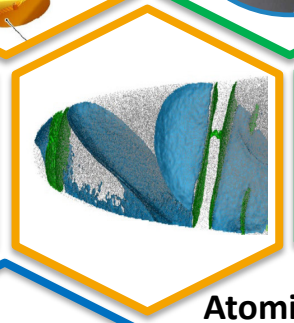


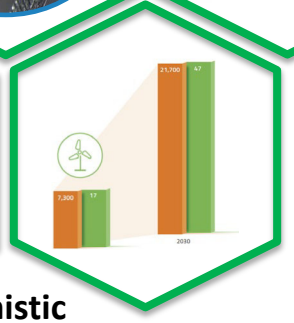




Magnetic imaging

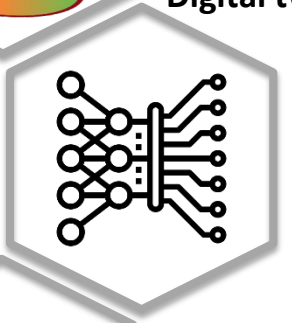






LCSA

Mlearning
Digital twins

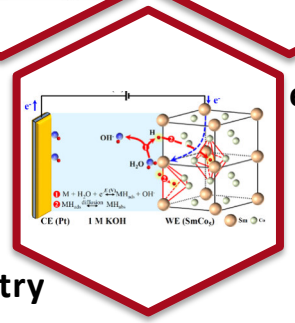


High entropy alloys

Soft magnets

Atomistic characterisation

Spin polarized electrochemistry



Spin-off

MAGNOTHERM®

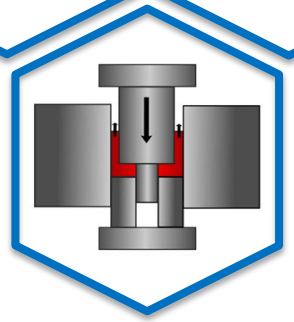
Additive manufacturing





Magnetic soft robotics

Advanced processing



FUNKTIONALE MATERIALIEN

FUNKTIONALE MATERIALIEN

TECHNISCHE UNIVERSITÄT DARMSTADT

Prof. Oliver Gutfleisch



“The energy transformation is a material transformation.”

☎ 06151 16 22140

oliver.gutfleisch@tu-darmstadt.de

http://www.mawi.tu-darmstadt.de/fm

https://scholar.google.de/citations?user=IMtVJ68AAAAJ&hl=de

ResearcherID: C-7241-2011

MATERIAL-
WISSENSCHAFT

TECHNISCHE
UNIVERSITÄT
DARMSTADT

EVONIK OPERATION GMBH

Standnummer 07

Evonik macht das Leben besser,
Tag für Tag.



17.11.2023 | Dr. Regina Fuchs-Winkler & Dr. Stephan Fengler

EVONIK
Leading Beyond Chemistry

Kein Produkt ist so perfekt,
dass man es nicht noch besser machen könnte.

spritsparendere	flauschigere	elastischere	gesündere	wirksamere



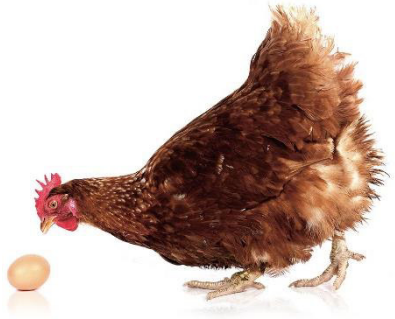
AUTOREIFEN



HANDTÜCHER



MATRATZEN



ERNÄHRUNG



TABLETTEN

EVONIK
Leading Beyond Chemistry

Dazu gehen
wir über die

CHEMIE

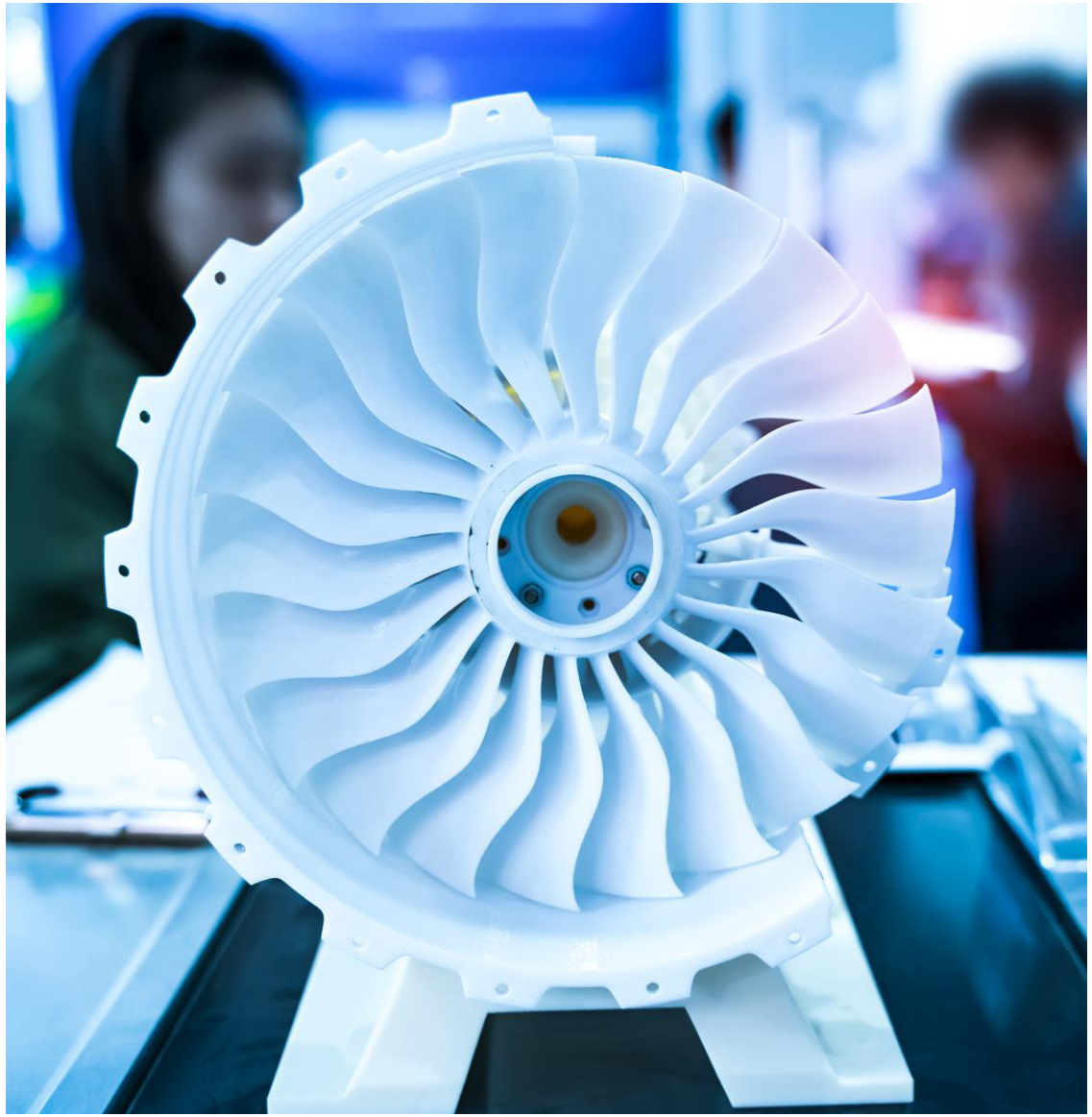
hinaus.

EVONIK
Leading Beyond Chemistry



So werden Batterien zu High-Performern, ...

EVONIK
Leading Beyond Chemistry



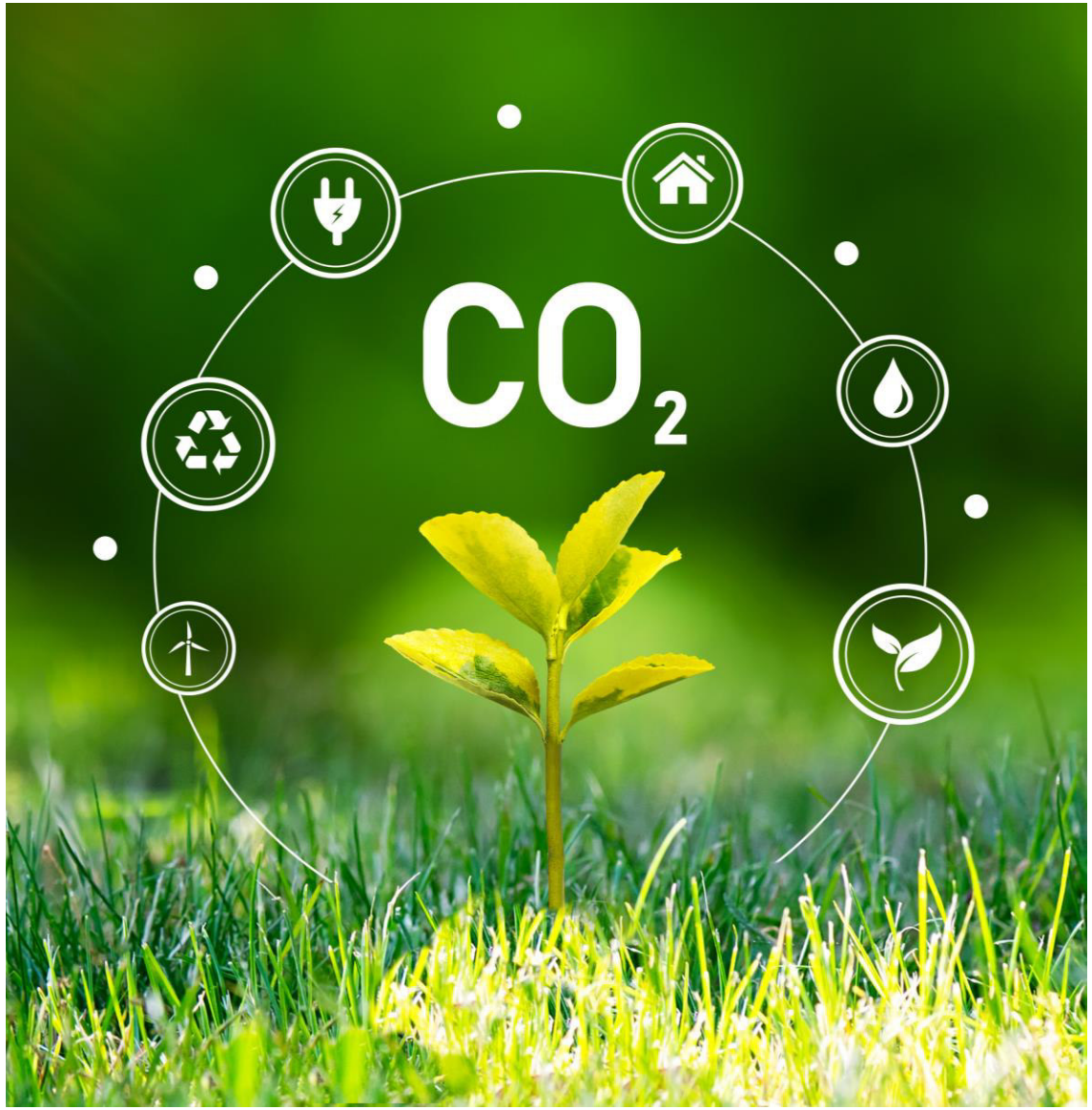
... 3D-Druck nachhaltiger, ...

EVONIK
Leading Beyond Chemistry



… Lipide zu Schutzschilden,…

EVONIK
Leading Beyond Chemistry



…und unsere Materialien zu CO_2 Fängern.

EVONIK
Leading Beyond Chemistry

Der Vorteil eines globalen Unternehmens - lokale Nähe (am Beispiel der Business Line Silica)







Hamina
Taavetti

Antwerp
Bonn
Hanau
Leverkusen
Oostende
Rheinfelden
Roussillon
Wesseling
Zubillaga - Lantaron

Charleston
Chester
Etowah
Havre de Grace
Mobile
Piscataway
Richmond
Waterford

Adapazari

Nanping
Shanghai
Qingdao
Zhenjiang

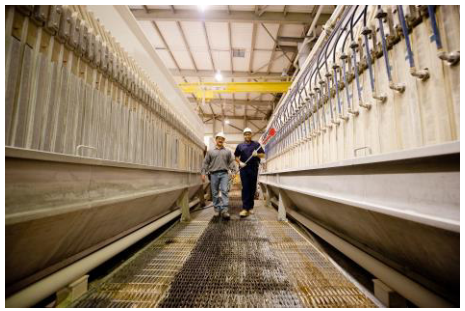
Seoul
Ako
Yokkaichi
Taoyuan

Map Ta Phut
Bangkok

Jhagadia
Mumbai



Americana



- Applied Technology
- Innovation/R&D
- Production, Fumed
- Production, Precipitated
- Production, Sodium Silicate

EVONIK
Leading Beyond Chemistry

LEADING BEYOND CHEMISTRY
TO IMPROVE LIFE, TODAY AND TOMORROW

EVONIK
Leading Beyond Chemistry


EVONIK
Leading Beyond Chemistry

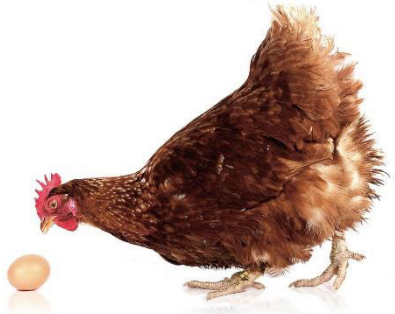
Evonik makes life better day in, day out.



17.11.2023 | Dr. Regina Fuchs-Winkler & Dr. Stephan Fengler

EVONIK
Leading Beyond Chemistry

No product is so perfect that you can’t improve it.

more fuel-efficient	fluffier	bouncier	healthier	more effective
				
TIRES	**TOWELS**	**MATTRESSES**	**NUTRITION**	**TABLETS**

EVONIK
Leading Beyond Chemistry

To make that happen,
we go beyond

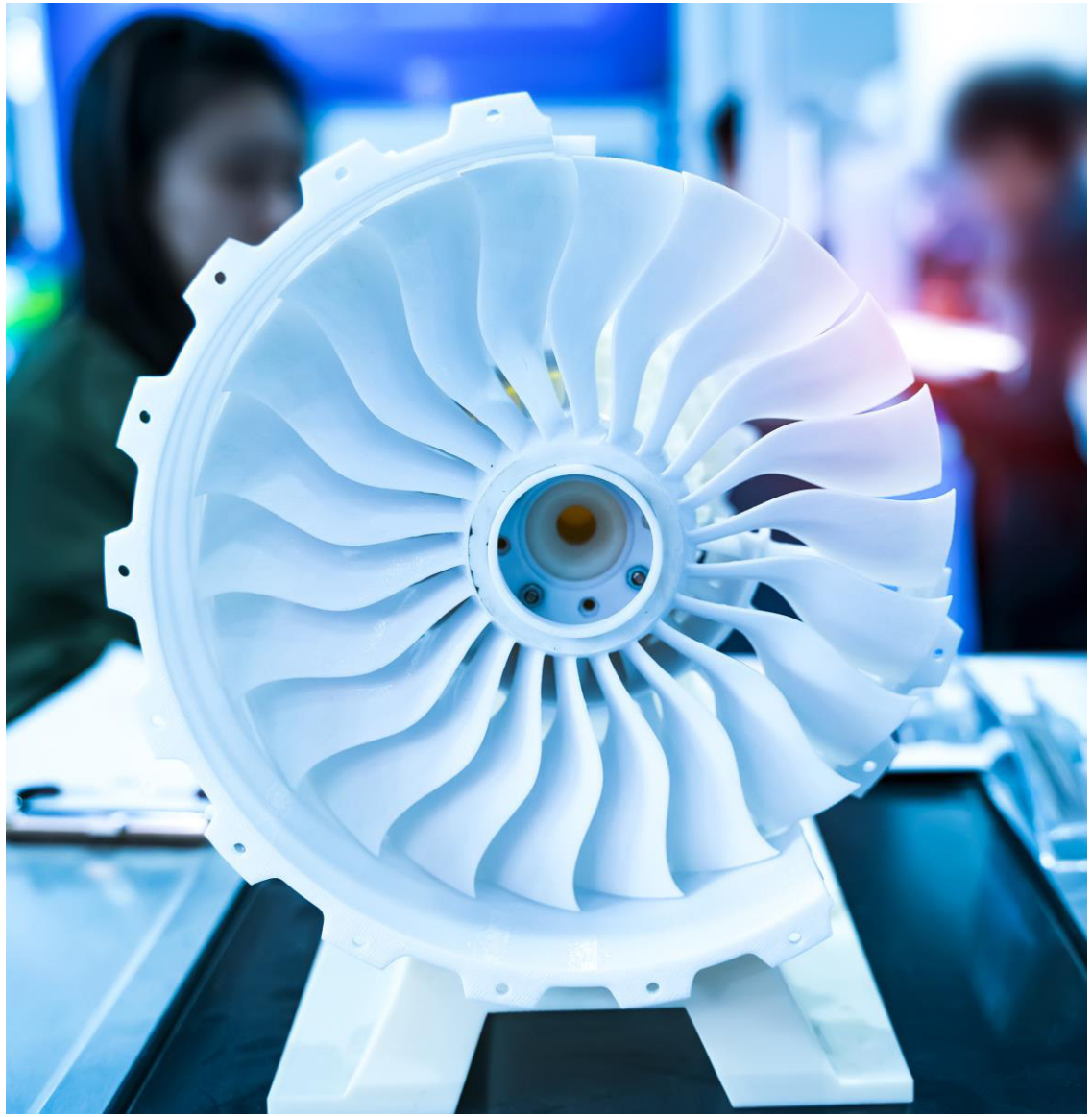
CHEMISTRY

EVONIK
Leading Beyond Chemistry



That’s how batteries become high performers, …

EVONIK
Leading Beyond Chemistry



… 3D printing turns more sustainable,

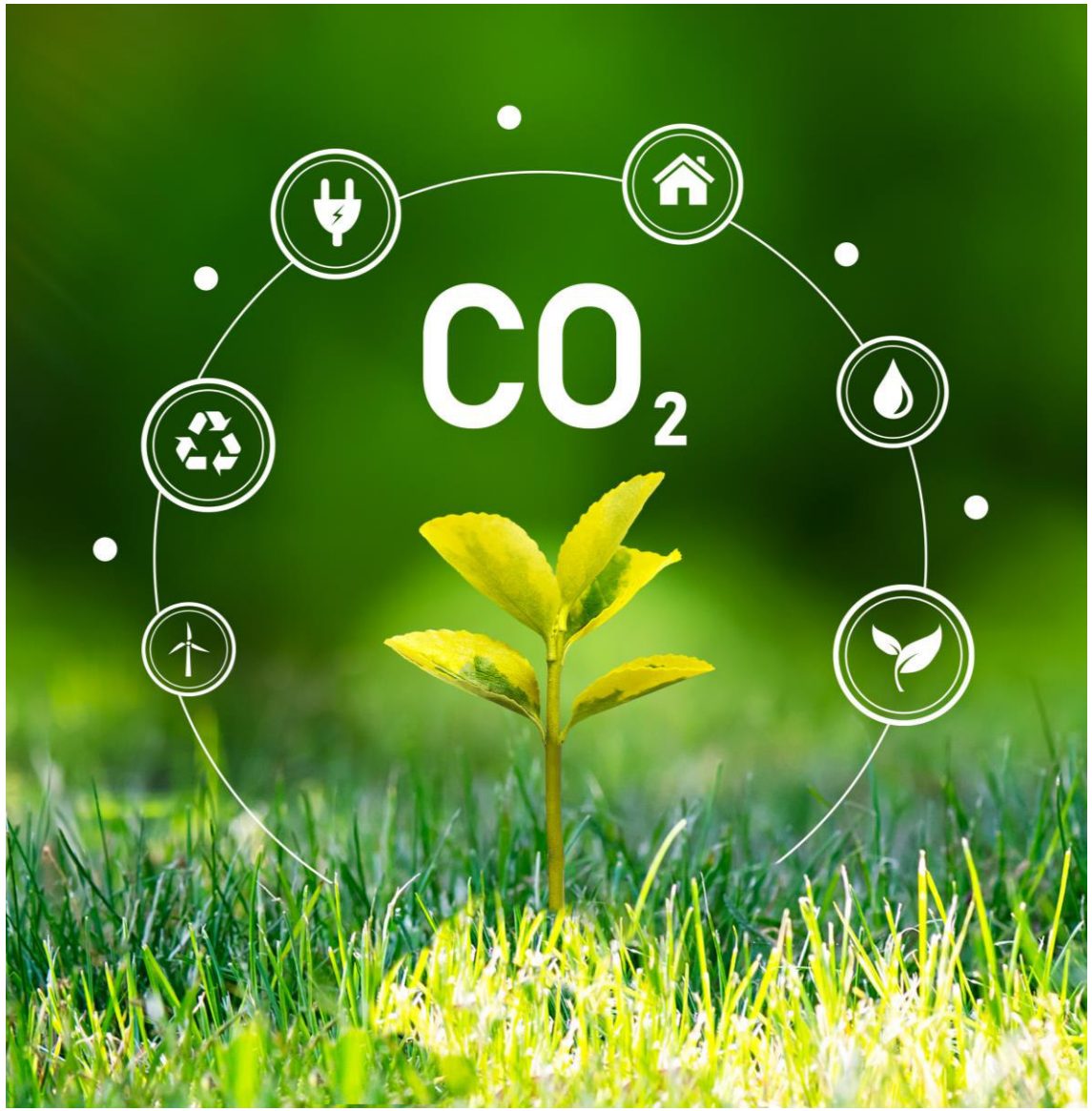
…

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… lipids become protective shields,

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Leading Beyond Chemistry



…and our materials used to capture CO_2.

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The advantage of a global enterprise – local proximity (e.g. Business Line Silica)







Hamina
Taavetti

Antwerp
Bonn
Hanau
Leverkusen
Oostende
Rheinfelden
Roussillon
Wesseling
Zubillaga - Lantaron

Charleston
Chester
Etowah
Havre de Grace
Mobile
Piscataway
Richmond
Waterford

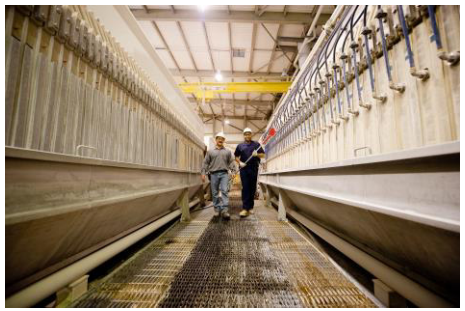
Adapazari

Nanping
Shanghai
Qingdao
Zhenjiang
Seoul
Ako
Yokkaichi
Taoyuan
Map Ta Phut
Bangkok

Jhagadia
Mumbai



Americana



Applied Technology
Innovation/R&D
Production, Fumed
Production, Precipitated
Production, Sodium Silicate

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LEADING BEYOND CHEMISTRY
TO IMPROVE LIFE, TODAY AND TOMORROW

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Leading Beyond Chemistry

MATERIAL-
WISSENSCHAFT

TECHNISCHE
UNIVERSITÄT
DARMSTADT

TU DARMSTADT – PHYSIKALISCHE METALLKUNDE

Standnummer 08



TECHNISCHE UNIVERSITÄT DARMSTADT

PHYSICAL METALLURGY

MaWi Industrietag

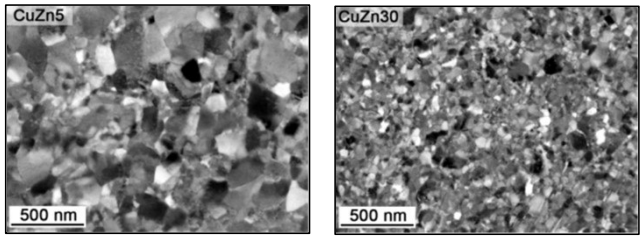
Prof. Dr.-Ing. Karsten Durst

Process –Microstructure - Properties

TECHNISCHE UNIVERSITÄT DARMSTADT

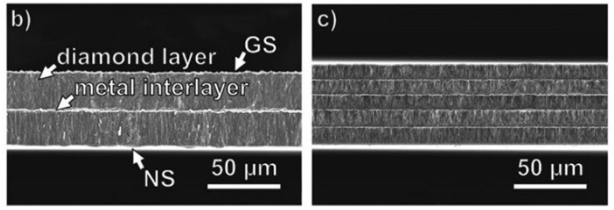
Nanostructured alloys by severe plastic deformation



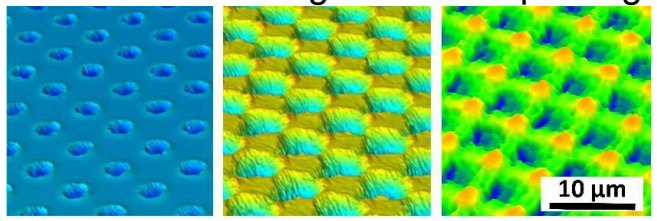




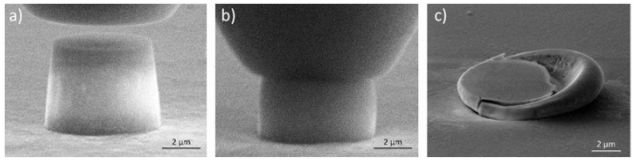
Thin films: Diamond laminate



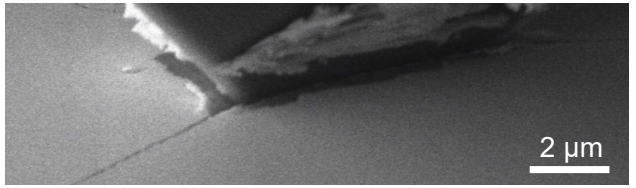
Surface structuring via nanoimprinting

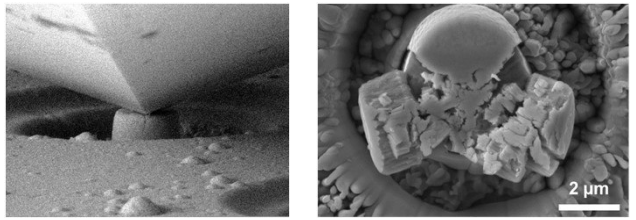


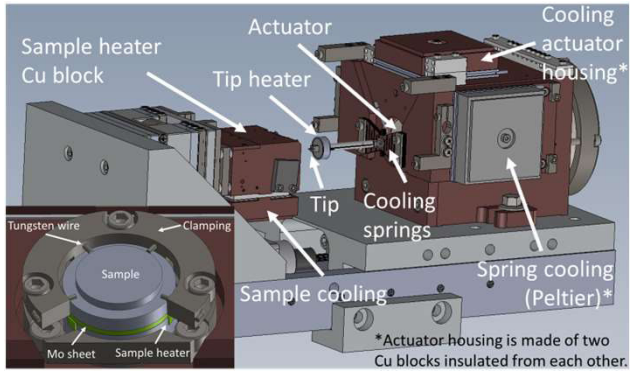
Electron-beam induced viscous flow in oxide glasses



In-situ and small-scale mechanical testing

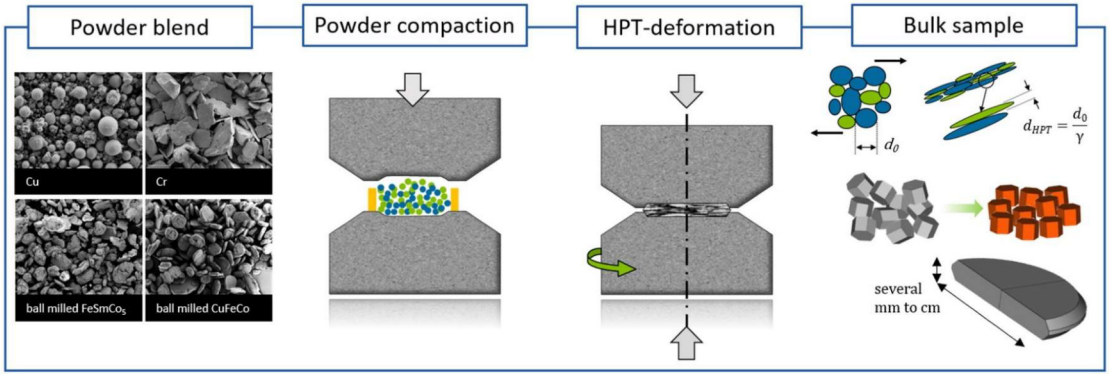


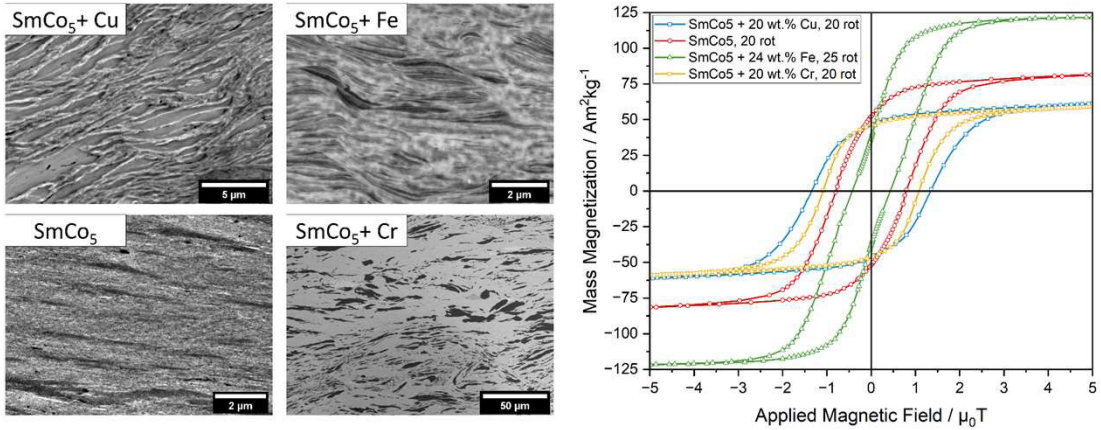




Nanostructured alloys via High Pressure Torsion

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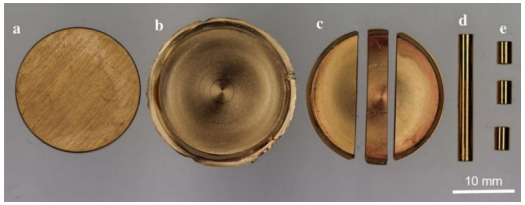


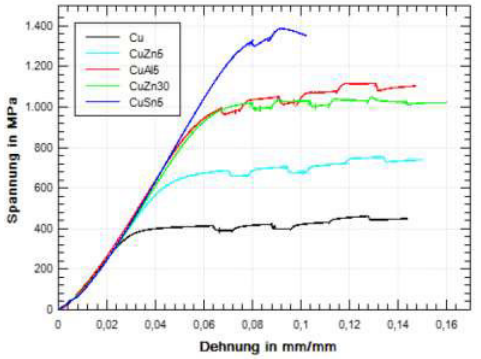


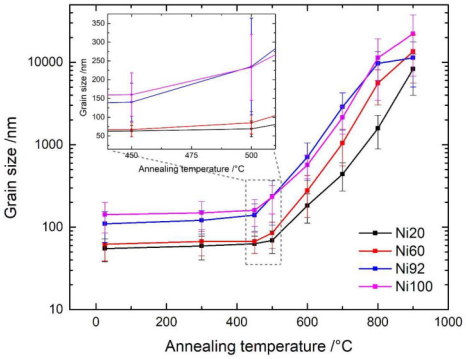
Hard **magnetic nanocomposites** beyond the phase diagram: SmCo5-X composites

Staab et al., Acta Mater (2023), Staab Mat Mater Trans (2023)

Bulk functional alloys







Enhanced strength, viscoplastic behaviour nanoscale plasticity, functionality

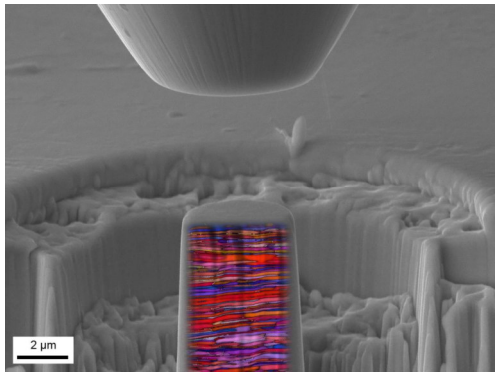
High Entropy Alloys: Cantor, Senkov Cu-X solid solutions

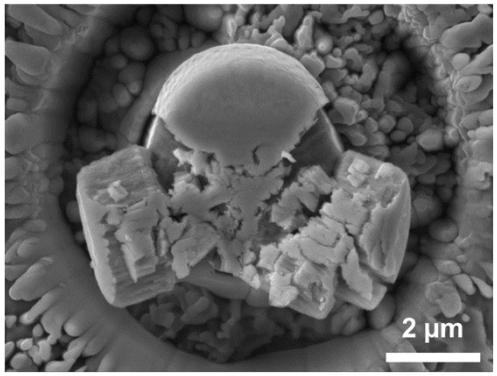
Keil et al., Acta Mater (2022), Keil et al Scripta Mat (2021)

In-situ and small-scale mechanical testing

Fracture mechanics, local property mapping, High Temperature behaviour up to 1100 C

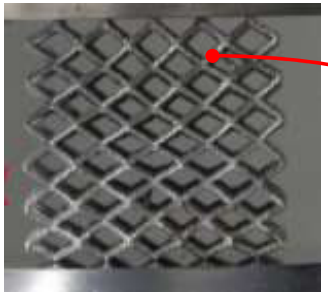
TECHNISCHE UNIVERSITÄT DARMSTADT



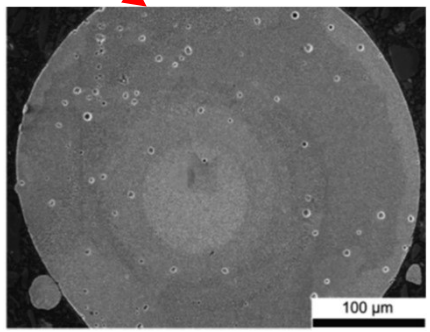


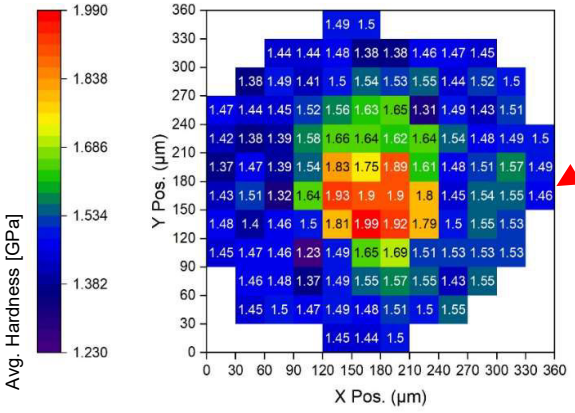
Pillar splitting tests (+FEA) for fracture toughness analyses
Pillar compression + EBSD

Bruns et al., Mater Des 227 (2020), 111796



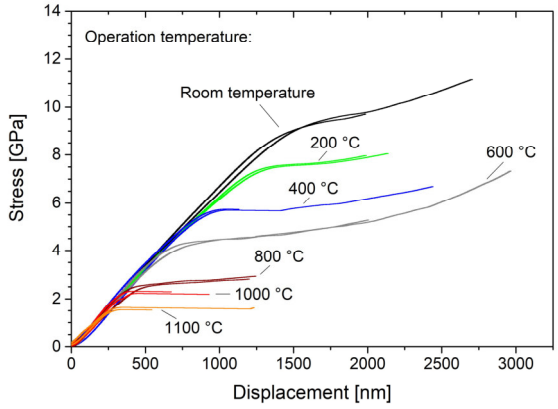
Local mechanical properties in AM lattice structures

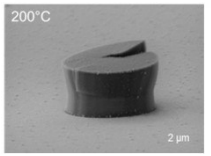


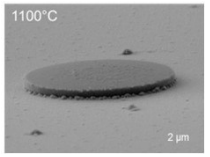


Sos et al., Mater Des 227 (2023), 111796

Flow stress SiO2, RT – 1100°

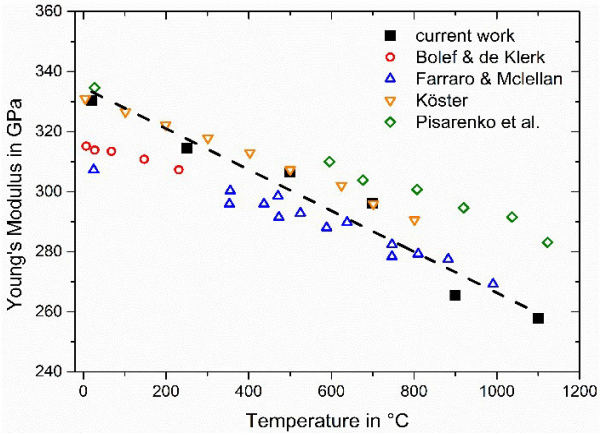






Bruns et al., Science Advances (2022),

Modulus Mo RT – 1100°

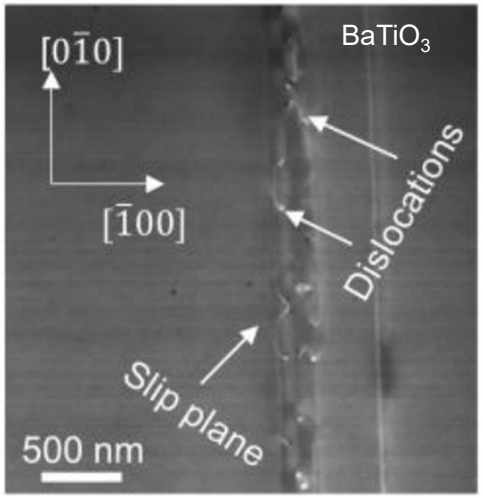


Minnert et al., Mater Des 192 (2020), 108727

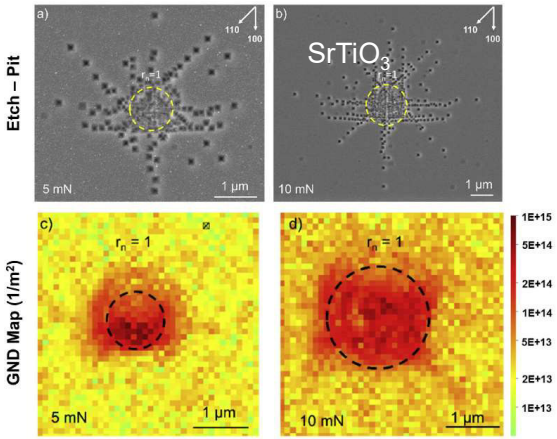
Deformation microstructures: Electron microscopy

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ECCI

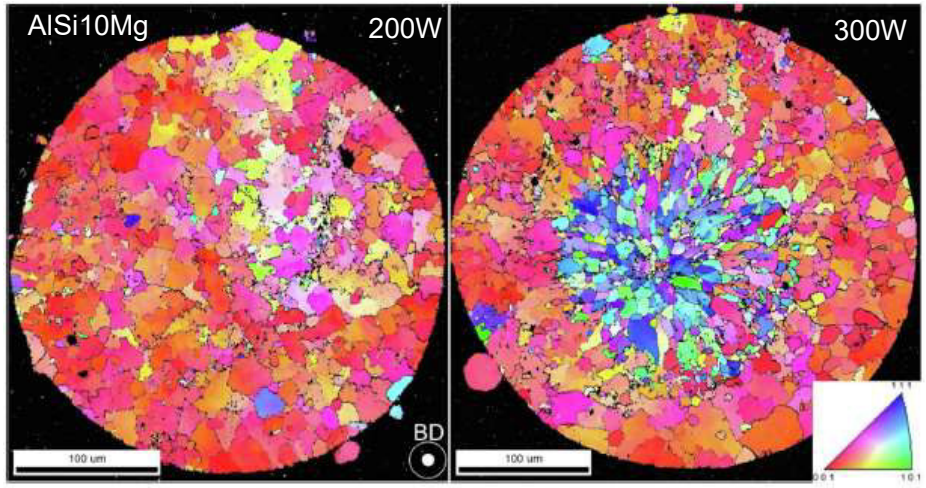


Höfling et al., Science 372 (2021), 961



Javaid et al., Acta Mater 139 (2017), 1

EBSD



Sos et al., Mater Des 227 (2023), 111796

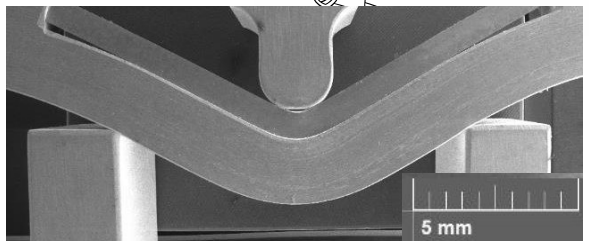
Microstructural evolution during and manipulation via additive manufacturing

Visualization and quantification of dislocations and **dislocation structures**

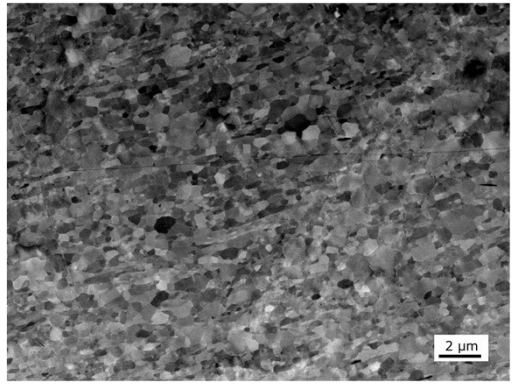
Micromechanical **in-situ testing** via bending stage

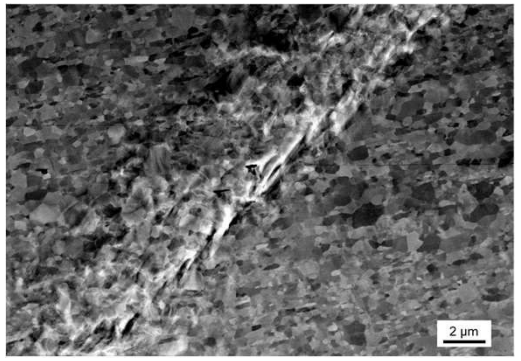
High resolution EBSD: GNDs

in-situ



Shear band formation





Physical Metallurgy

Interested -> meet us @ stand 08

TECHNISCHE UNIVERSITÄT DARMSTADT



Prof. Dr.-Ing. Karsten Durst

Dr.-Ing. Enrico Bruder
Dr.-Ing. Sebastian Bruns
Group leader





VACUUMSCHMELZE GMBH & CO. KG

Standnummer 09

VACUUMSCHMELZE

Ihr Partner für hochentwickelte magnetische Lösungen



170+
Legierungen

500+
Patente

4.300+
Mitarbeiter

5 Standorte

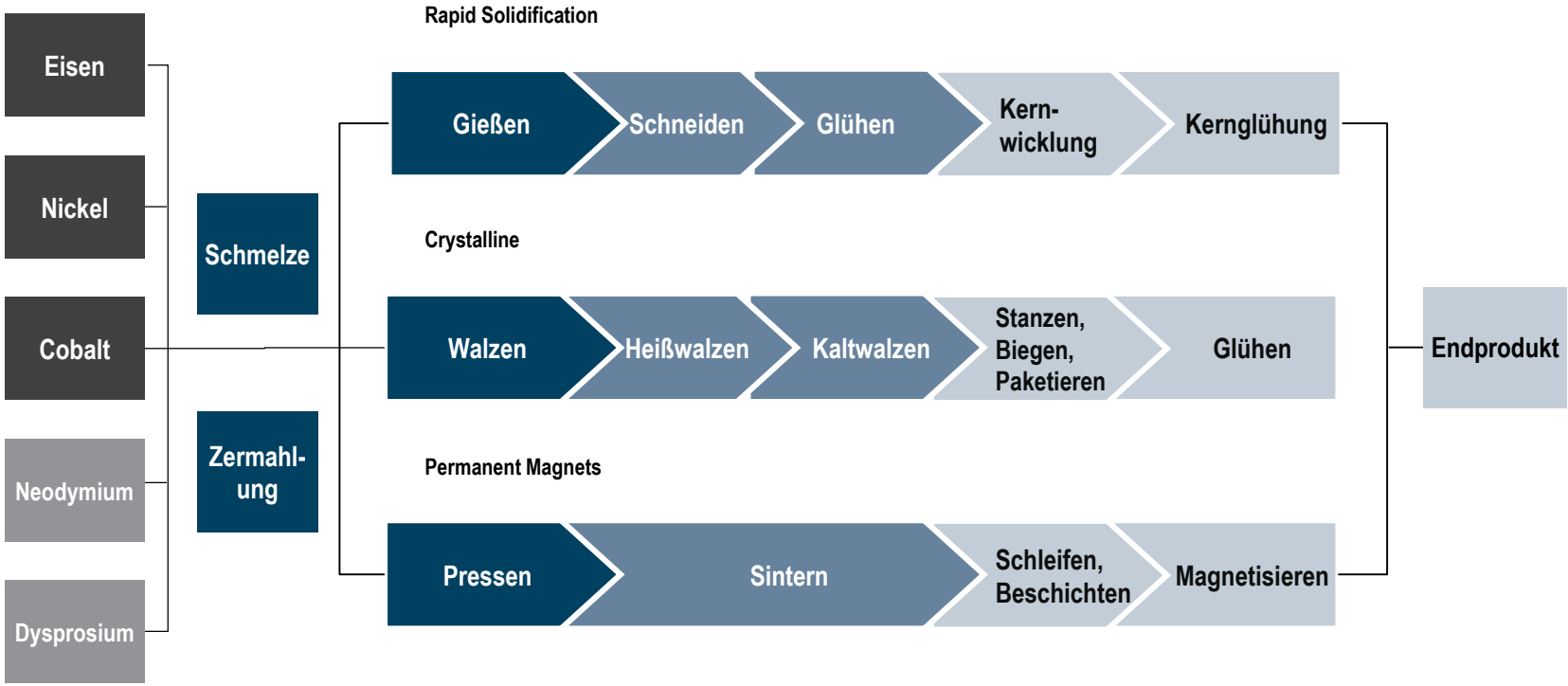
500+
Kundenspezifische Lösungen

2.000+
Aktive Kunden

Der Magnetismus ist unsere Heimat

Wir sind einer der führenden Hersteller von magnetischen Legierungen und daraus veredelten Produktlösungen.

- Durch das Schmelzen im Vakuum stellen wir Legierungen höchster Reinheit auf Basis von Fe, Co und Ni her.
- Die VAC ist Europas führender Hersteller von Permanentmagneten aus seltenen Erden.









Leistungsstarke Produktlösungen für vielfältige Anwendungen

	Kristallines Material	Kristalline Stanzteile	Stromsensoren	Nanokristallines Material	Kerne und Bauelemente	Dauermagnete und Systeme
Produktlösung	Band aus Nickeleisen 	Blechpakete aus Kobalteisen 	(Differenz-) Stromsensoren 	Nanokristallines Band 	Stromwandler 	Magnetsysteme 
Anwendung	Magnetische Sensorik und Abschirmung 	Elektrische Hochleistungsmotoren 	Elektrische Sicherheit 	Drahtloses Laden 	Elektrische Installationssicherheit 	Positionssensoren 
Branche	Automotive Luftfahrt Industrie Forschung	Motorsport Luftfahrt Industrie	eMobility-Ladeinfrastruktur Erneuerbare Energien Industrie	Smartphones Tablet PC's	Elektrische Installation	Automotive Industrie Forschung

Bereich Forschung und Entwicklung

180+
R&D Mitarbeiter

Umfangreiche
Charakterisierungs-methoden

Vielfältige
Forschungskooperationen

Aktuelle Themen und Fragestellungen:

- Machine Learning unterstützte Materialographie
- Textureinstellung an kristallinen Werkstoffen
- Additive Fertigung von weichmagnetischen Werkstoffen



VACUUMSCHMELZE

Ihr Partner für hochentwickelte magnetische Lösungen

ADVANCED MAGNETIC SOLUTIONS

MATERIAL-
WISSENSCHAFT

TECHNISCHE
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DARMSTADT

TU DARMSTADT – MATERIALS & RESOURCES

Standnummer 10



RESEARCH GROUP MATERIALS & RESOURCES

Prof. Dr. Anke Weidenkaff

© Thomas Ott

SUSTAINABLE MATERIALS FOR SUSTAINABLE ENERGY CONVERSION

TECHNISCHE UNIVERSITÄT DARMSTADT

Fraunhofer IWKS

Thermoelectric materials

Lithium ion battery recycling

Green²ICT materials

Lead-free photovoltaics

Photoanode materials for solar water splitting



Biowaste to chemicals

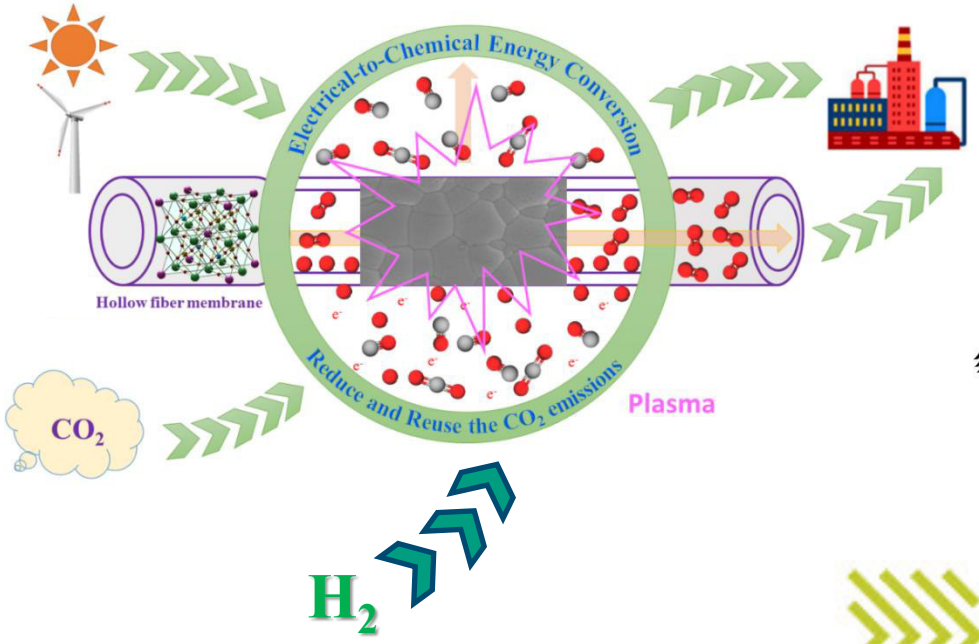
Pyrolysis / plasmolysis of waste plastic

CO_2 utilization

Oxygen transport membrane

Solid oxide fuel cell / solid oxide electrolysis cell materials

OXYGEN TRANSPORT MEMBRANES



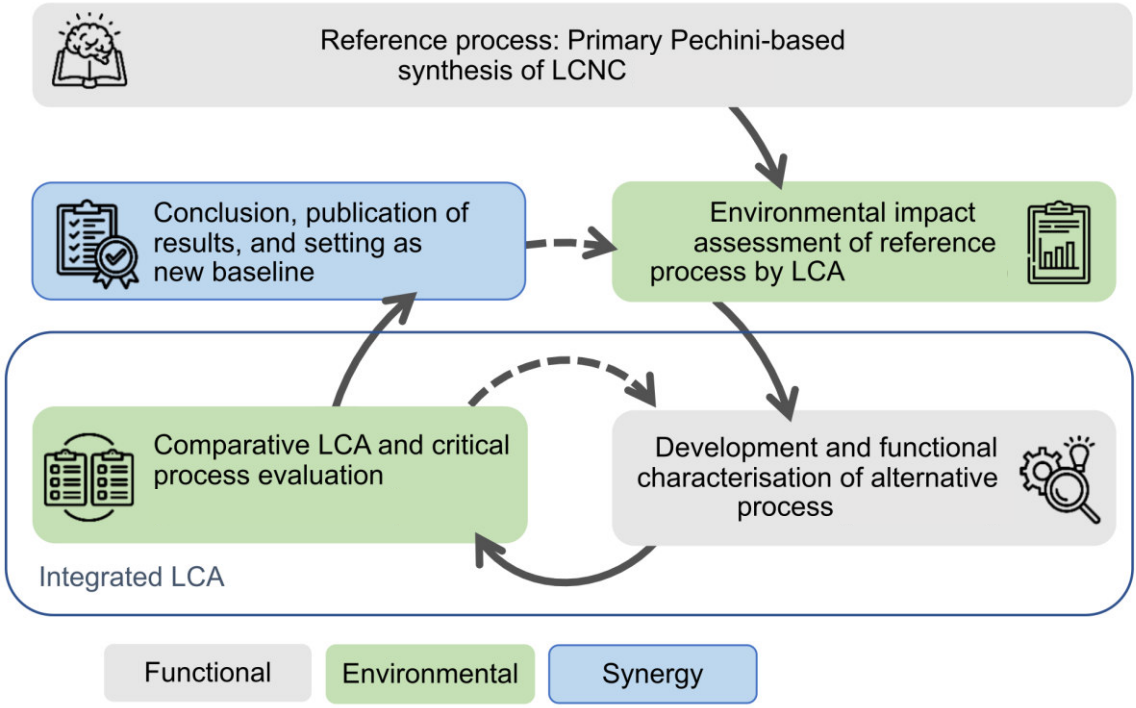
SPONSORED BY THE

Federal Ministry of Education and Research

Wasserstoff Leitprojekte

Grün. Groß. Global.

Approach of integrating early-stage LCA into chemical process development



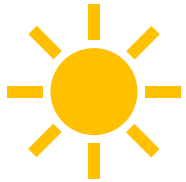
- ✓ Microwave-assisted plasma conversion process of CO_2 & H_2 to form CH_3OH
- ✓ Oxygen transport membrane (OTM) needed for $p(O_2)$ control

- – Because of entropy recycling is not for free!
- – Recycling requires energy and/or chemical input
- ✓ Environmental impacts need scientific analysis

THERMOELECTRIC CONVERSION

Or using entropy

direct conversion



Seebeck effect

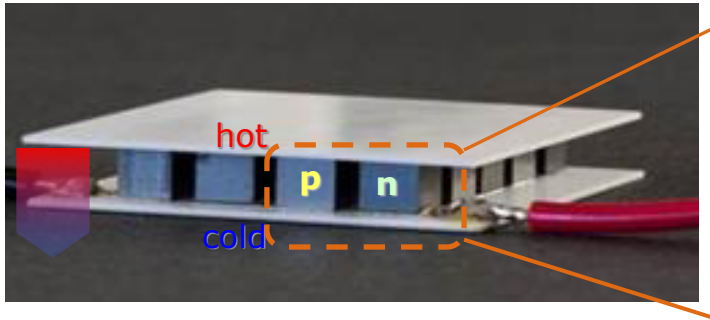


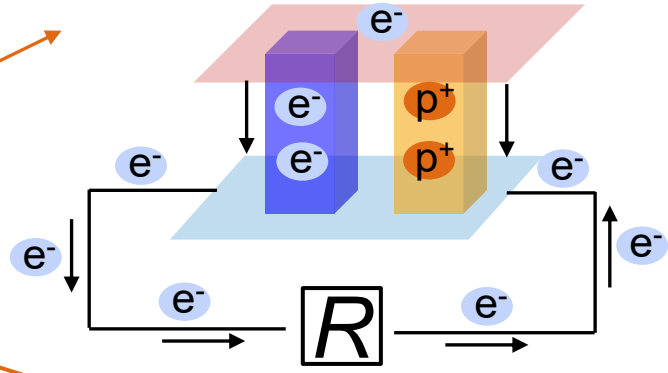


Electricity

Heat Peltier effect

Thermoelectric generator





SAVE THE DATE

Fraunhofer IWKS

Fraunhofer Research Institution for Materials Recycling and Resource Strategies IWKS

PRESS & MEDIA CAREER DEUTSCH

ABOUT US COMPETENCIES PROJECTS EVENTS PUBLICATIONS



MATERIAL-
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UNIVERSITÄT
DARMSTADT

LEISTUNGSZENTRUM „GREEN MATERIALS FOR HYDROGEN“

Standnummer 11

17.11.2023

Leistungszentrum „Green Materials for Hydrogen“

04.10.2023



Fraunhofer

Green Mat 4 H_2 Leistungszentrum

Das Leistungszentrum
GreenMat4H_2

Leistungszentrum GreenMat4H_2 auf einen Blick

Wir erforschen und entwickeln **„grüne“ Werkstoffe** und **Technologien** zur sicheren **Herstellung, Speicherung, Transport und Nutzung von Wasserstoff** und für die Umstellung bestehender Strukturen auf Wasserstoffanwendungen

Ziele:
Eine nachhaltige und zuverlässige Wasserstoff-Kreislaufwirtschaft in Hessen realisieren und damit einen wichtigen Beitrag zum Klimaschutz leisten; Stärkung von Hessen als Hochtechnologieland;

Unser Anspruch:
Zentrale Anlaufstelle für die Wasserstoff-Wirtschaft im Rhein-Main-Gebiet sowie darüber hinaus; Materialkreisläufe der H_2-Wirtschaft nachhaltig schließen

Green Mat 4 H_2 Leistungszentrum



 © Fraunhofer I Leistungszentrum-Wasserstoff Hessen

Fraunhofer

Beteiligte Institute

GreenMat4H$_2$



Fraunhofer IWKS (Hanau)

Nachhaltige Materialien | Plasmalyse | Kreislaufkonzepte | Recyclingtechnologien | systemische Betrachtung der ökonomischen und ökologischen Auswirkungen



Fraunhofer LBF (Darmstadt)

Bewertung der Sicherheit und Zuverlässigkeit von H_2-Systemen | Optimierung und Lebensdauerbewertung von Werkstoffen und Komponenten | Entwicklung von acoustic emission basierter Sensorik als Monitoringsystem für Wasserstofftanks | FMEA

© Fraunhofer I Leistungszentrum-Wasserstoff Hessen

Kooperationsmöglichkeiten

GreenMat4H_2

- Zugang zu einem breiten Spektrum an maßgeschneiderten Lösungen im Rahmen von Auftragsforschungsprojekten
- Gemeinsame öffentlich geförderte Projekte; Unterstützung bei der Zusammenstellung des Konsortiums und der Antragsstellung
- Zugang zu Know-how aus Hochschulen und der Fraunhofer-Welt zur schnellen Markteinführung von Forschungsergebnissen
- Gezielte IP-Strategie und Unterstützung bei Patentierung und Lizensierung
- Nutzung von Open Labs / Testlabs zur Validierung und Verifizierung von Technologieentwicklungen
- Personalaustausch und Realisierung gemeinsamer Beschäftigungsmodelle von Fachexperten → Job-Sharing-Modelle für erhöhte Effizienz und Synergiebildung
- Lern- und Weiterbildungsangebote

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Themenschwerpunkte

GreenMat4H_2



Plasmalyse
Elektroden und Membranen
Nachhaltige Materialien für SOFC/SOEC



Materialentwicklung
Kunststoffe

Betriebsfestigkeit von Komponenten der Wasserstoffwirtschaft & E-Mobilität



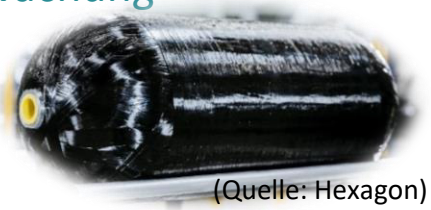
H_2 Erzeugung

H_2 Transport/ Speicherung

H_2 Nutzung

Green Mat 4 H_2 Leistungszentrum

Sensorgestützte Strukturüberwachung



(Quelle: Hexagon)





Kreislaufwirtschaftskonzepte:
Brennstoffzellen, Elektrolyseure, H_2-Tanks



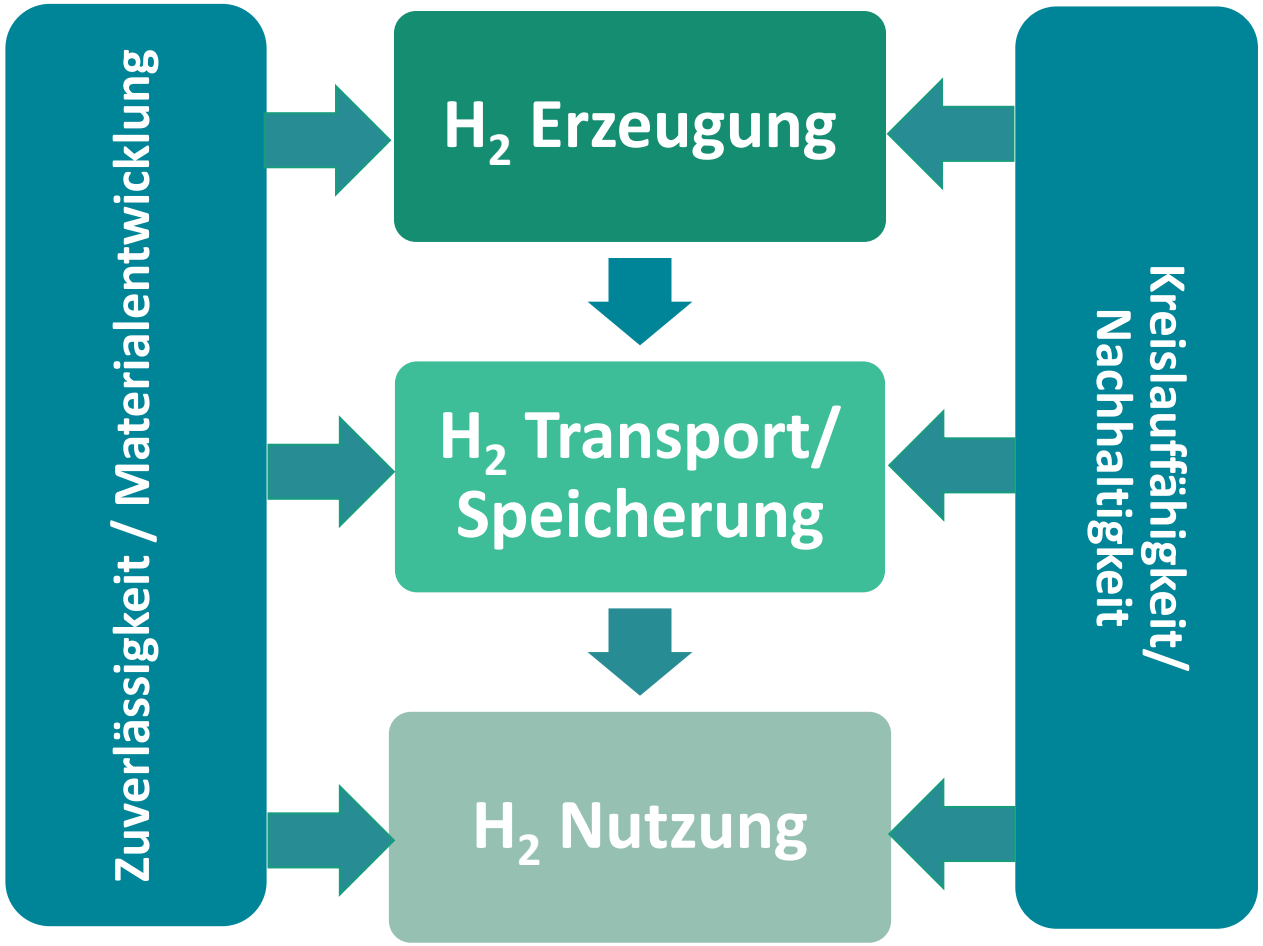
Ermüdungsprüfung in gasförmigem Medium (H_2, N_2)

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Fraunhofer

Themenschwerpunkte

GreenMat4H_2



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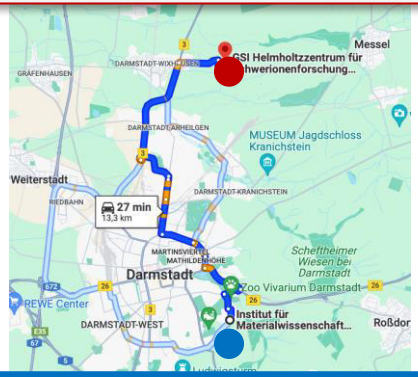
TU DARMSTADT & GSI MATERIALFORSCHUNG – IONENSTRAHLMODIFIZIERTE MATERIALIEN,

Standnummer 12

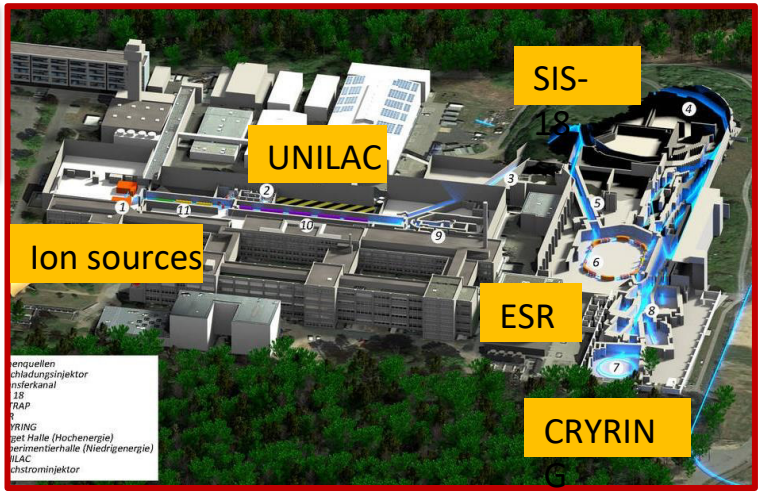
14.11.2023

Bestrahlungsanlagen für die Ionenstrahlmodifizierung von Materialien und Strahlungshärteprüfungen

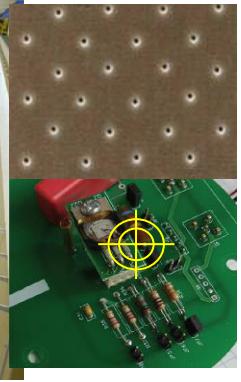
GSI Helmholtzzentrum für Schwerionenforschung
Materialforschung











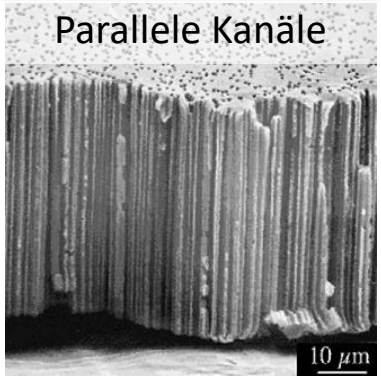


UV/VIS, IR, Raman,SIMS,SEM, XRD,…

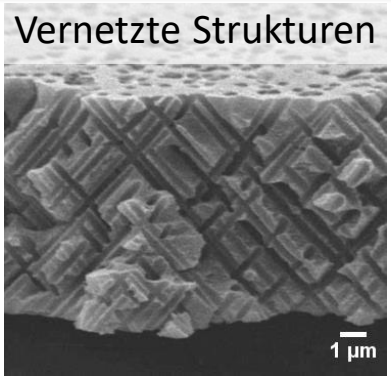
FB Material- und Geowissenschaften
FG Ionenstrahlmodifizierte Materialien

Ionenspur-Nanotechnologie: von selektiven Filtern… bis zu hochempfindlichen Sensoren und Energiematerialien

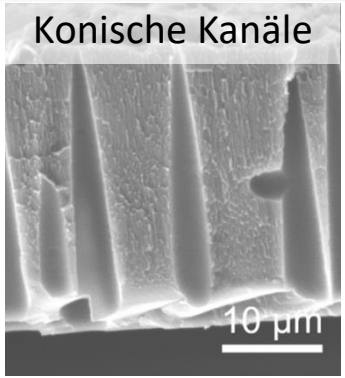
Parallele Kanäle



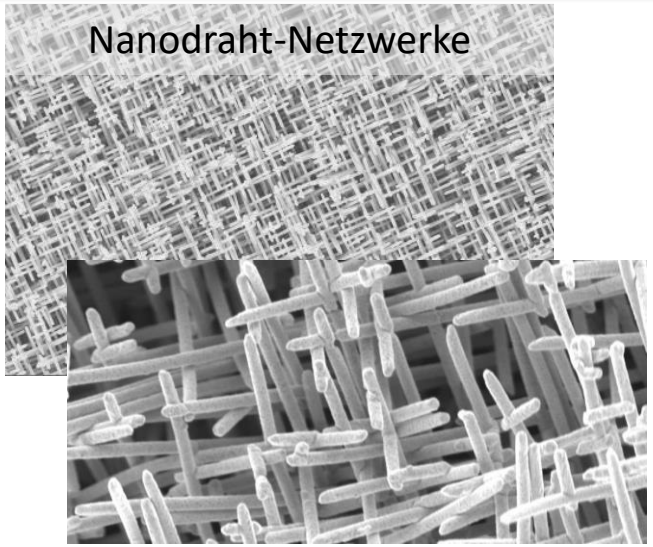
Vernetzte Strukturen



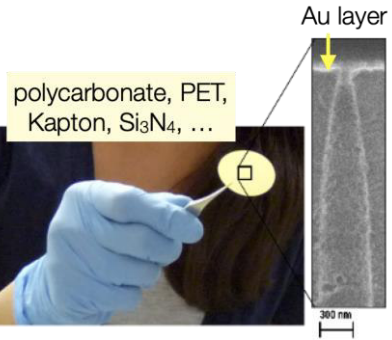
Konische Kanäle

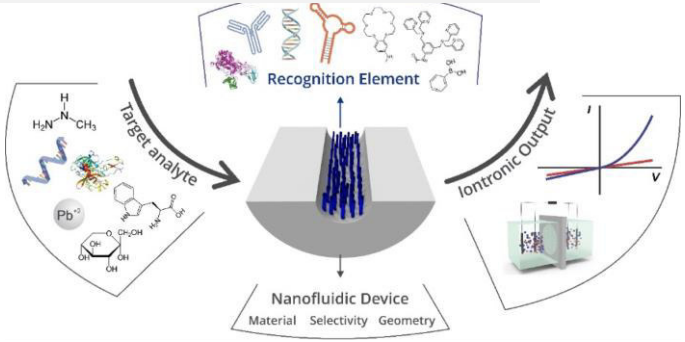


Nanodraht-Netzwerke



Selektiv und hochempfindliche Sensoren





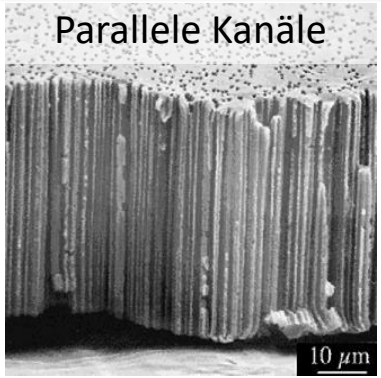
Anwendungsbereiche: Batterien, Katalyse, Brenstoffzellen, Sensorik, …

TECHNISCHE UNIVERSITÄT DARMSTADT

Ionenspur-Nanotechnologie: von selektiven Filtern… bis zu hochempfindlichen Sensoren und Energiematerialien

FAIR GSI

Parallele Kanäle



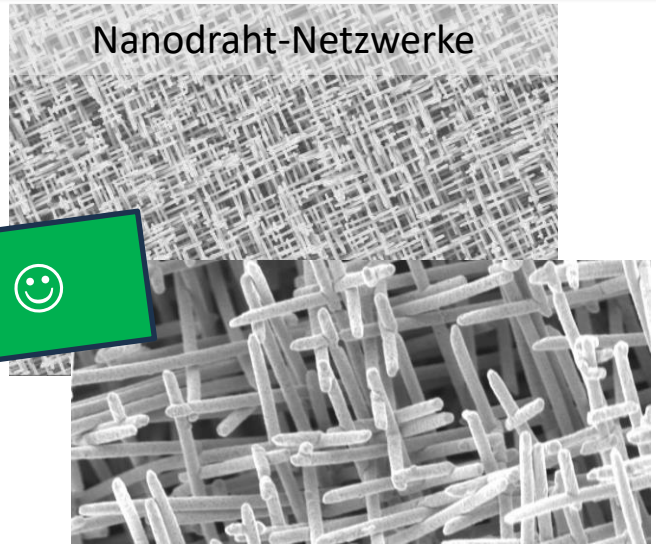
Vernetzte Strukturen



Konische Kanäle

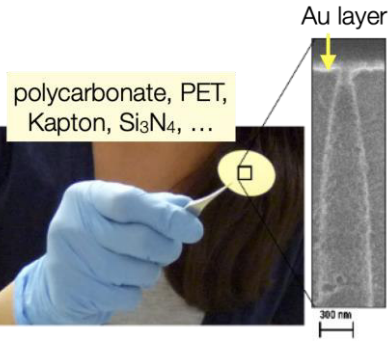


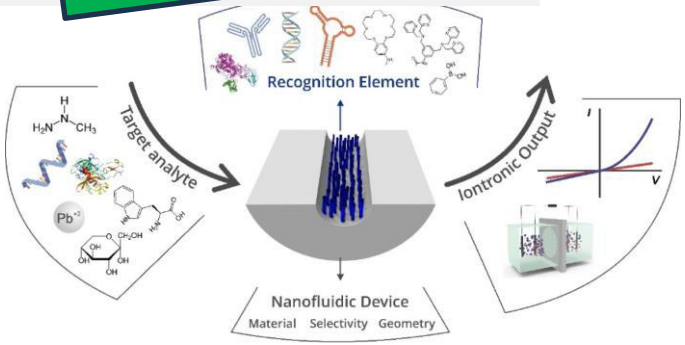
Nanodraht-Netzwerke



Wir sehen uns am Stand 12 ☺

Selektiv und ho… …ensoren





Anwendungsbereiche: Batterien, Katalyse, Brenstoffzellen, Sensorik, …

MATERIAL-
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DARMSTADT

UMICORE AG & CO. KG

Standnummer 13

Introducing Umicore

Unique business model

INTERNAL DRIVER

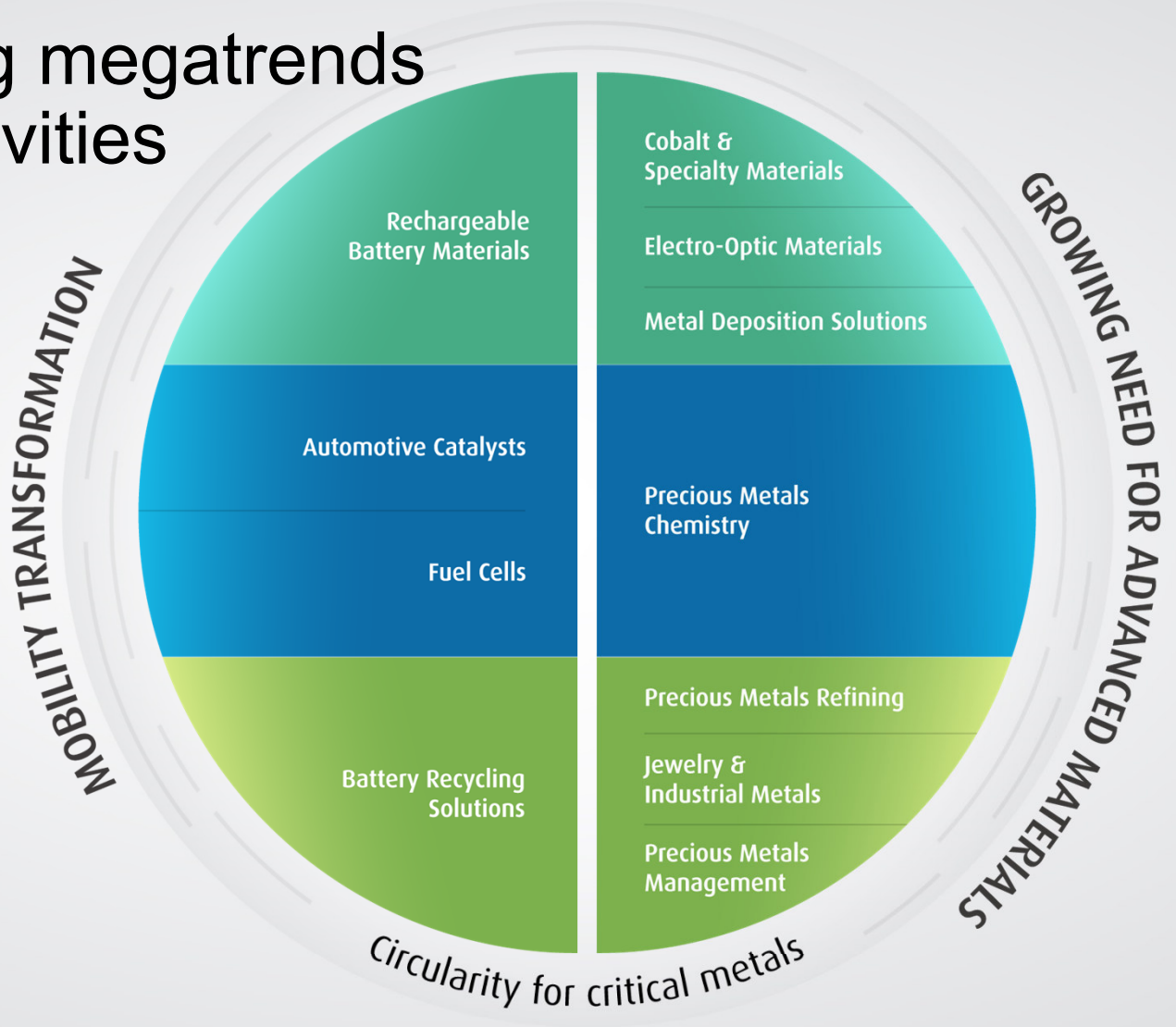


Supportive megatrends

EXTERNAL DRIVER

Industry **leader** in sustainability

Accelerating megatrends drive all activities



umicore

ENERGY & SURFACE TECHNOLOGIES

CATALYSIS

RECYCLING

MATERIAL-
WISSENSCHAFT

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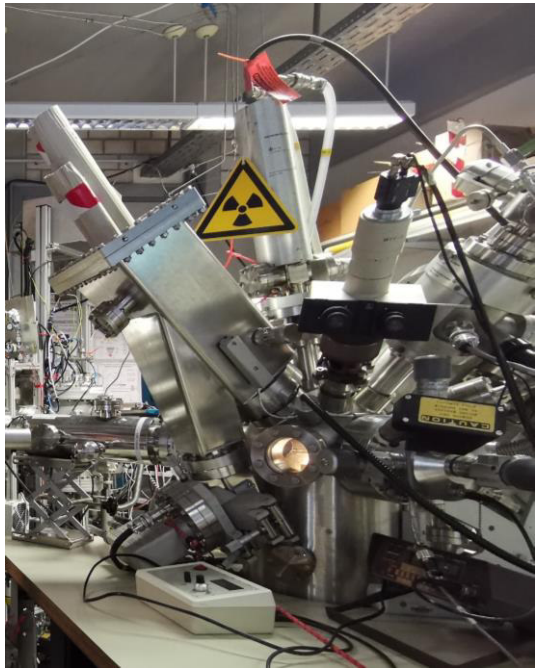
TU DARMSTADT – ELEKTRONENSTRUKTUR VON MATERIALIEN

Standnummer 14

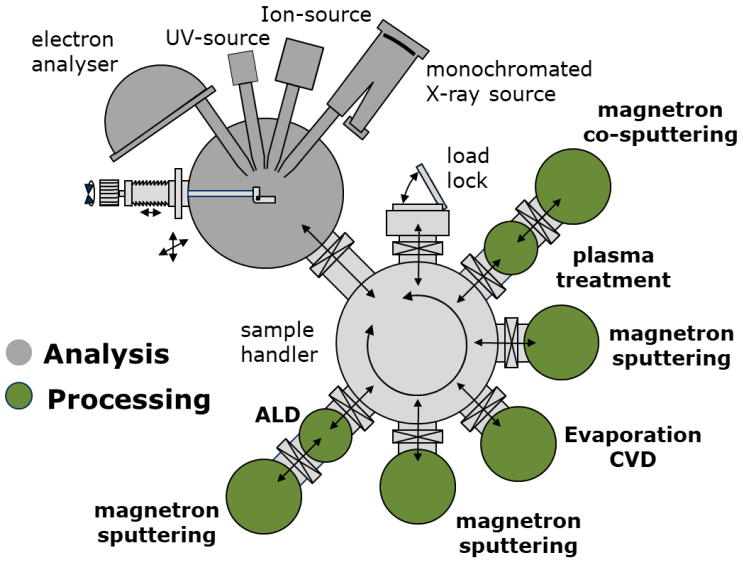
Electronic Structure of Materials

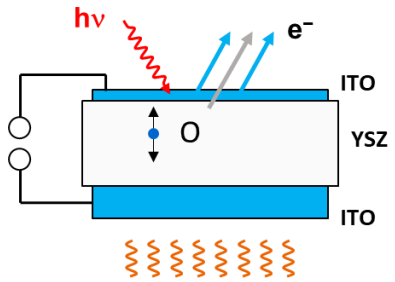
Analysis of defect properties of oxides and their relation to functional properties

XPS with in-situ sample and thin film processing



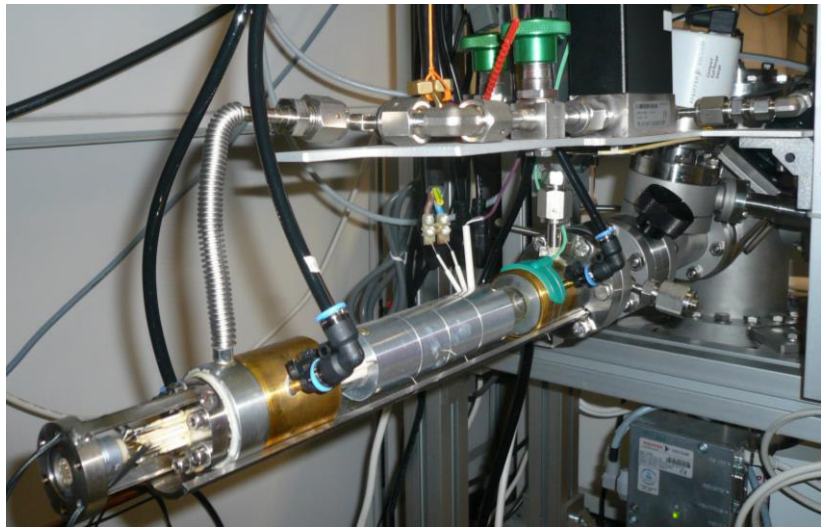
- surface chemistry
- Surface potentials





Electrochemical cell setup

Electrical analysis in controlled atmosphere

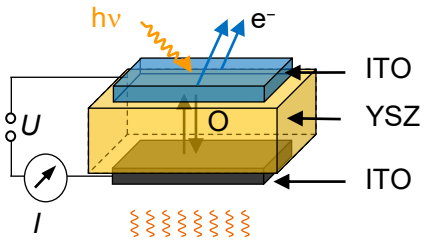


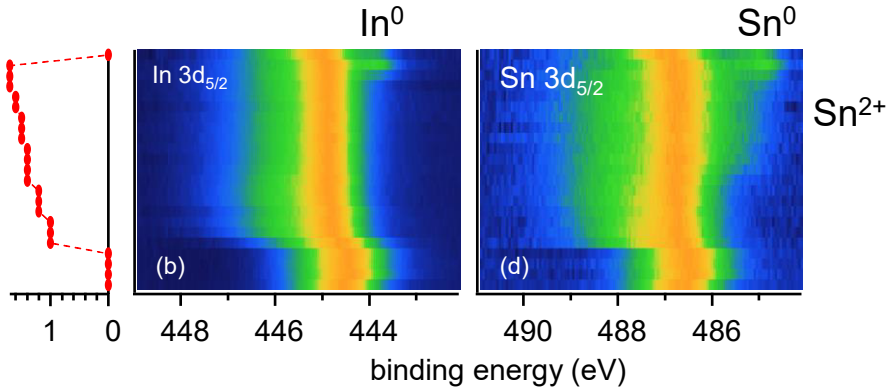
- Electrical conductivity
- Defect equilibria
- Diffusion coefficients

Research on Electroceramic Oxides

TECHNISCHE UNIVERSITÄT DARMSTADT

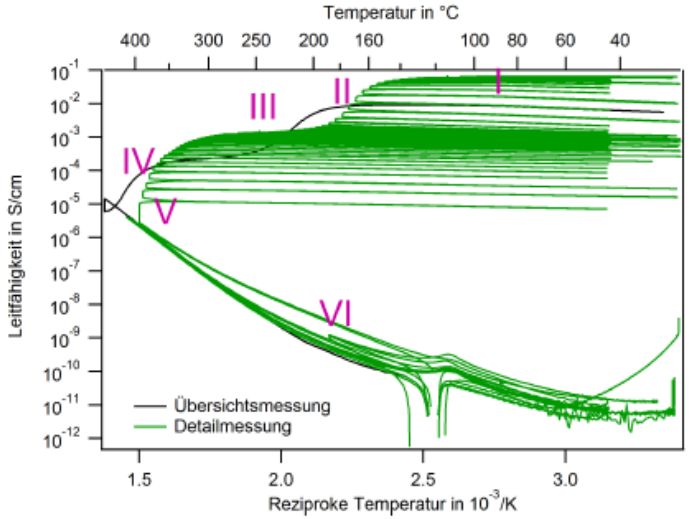
- **Electrical conductors**
  - Doping and conductivity limits
  - Influence of grain boundaries
  - In_2O_3 (previously also SnO_2, ZnO)





- **Piezoelectric and dielectric perovskites**
  - Influence of charges on (di-)electric and interface properties
  - $BaTiO_3$, $NaNbO_3$, $Pb(Zr,Ti,Sn)O_3$, $Pb(Mg_{1/3}Nb_{2/3})O_3$, $BiFeO_3$

- **Mixed ionic electronic conductors**
  - Charge compensation mechanisms and valence changes
  - $(La,Sr)(Fe,Co,Mn)O_3$



Collaborative Research Center FLAIR

ESM TECHNISCHE UNIVERSITÄT DARMSTADT

Fermi level engin-eering

Composition

Processing



Empirical evolutionary development

FLAIR

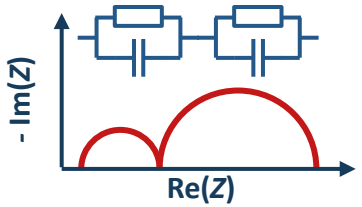
Predictable properties

Revolutionary development

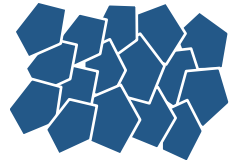


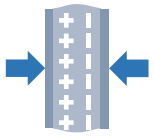
Properties

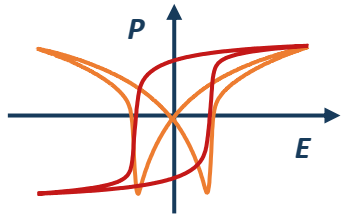












Thinking materials development differently

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DARMSTADT

HESSEN TRADE & INVEST GMBH

Standnummer 15

HESSEN TECHNOLOGIELAND HESSEN

VERNETZT. ZUKUNFT. GESTALTEN.

technologieland-hessen.de

WILLKOMMEN IM **TECHNOLOGIELAND HESSEN**

Informieren. Beraten. Vernetzen.

Hessisches Ministerium für Wirtschaft, Energie, Verkehr und Wohnen

Projektträger:
Hessen Trade & Invest GmbH

HESSEN

TECHNOLOGIELAND HESSEN

Publikationen



Fachveranstaltungen



Informationsplattform



Beratung



Kooperationen



materials valley

Messebeteiligungen



formnext

Frankfurt am Main, 07.–10.11.2023

HESSEN TECHNOLOGIELAND HESSEN

Förderprogramme

F&E-Förderung



Die Förderung für **innovative Forschungs- und Entwicklungsvorhaben** von **kleinen und mittleren Unternehmen.**

Fokus auf innovative Technologien - offen für alle Themen und Branchen.

LOEWE-Förderlinie 3

LOEWE
Exzellente Forschung für Hessens Zukunft

Die **LOEWE-Förderlinie 3** ist das themenoffene Angebot zur Förderung von **technologie-orientierten Forschungs- und Entwicklungsprojekten** von Unternehmen **in Kooperation** mit Hochschulen oder Forschungseinrichtungen.

PIUS-Invest



Das Programm **PIUS-Invest** bezuschusst Investitions-projekte, die die **Ressourcen-effizienz verbessern und CO2-Emissionen einsparen**.

Ressourcenwendepaket



Die **FuE-Förderung für eine effiziente Kreislaufwirtschaft:** Vorhabenförderung zur Entwicklung von Technologien zum Schließen von Stoffkreisläufen, Erhöhung des Rezyklateinsatzes sowie Lösungen für eine Kreislaufwirtschaft.

Stellen Sie jetzt einen Antrag!



Klimaplan Hessen 2030

Ressourcenwendepaket - F&E-Förderung für effiziente Kreislaufwirtschaft

Industriellen Forschung oder der **experimentellen Entwicklung** (**TRL 4-8**) im Bereich
- **Schließen von Stoffkreisläufen** (Sortier- und Recyclingtechnologien)
- **Erhöhung des Rezyklateinsatzes**
- Übergang zu einer **Kreislaufwirtschaft**

Projektkosten **mind. 100k EUR** für **max. 3 Jahre** bei **industrieller Forschung bis zu 50 Prozent** förderfähig. Bei der **experimentellen Förderung**:
- bis zu 45 Prozent bei kleineren Unternehmen (weniger als 50 Mitarbeiter)
- bis zu 35 Prozent bei mittleren Unternehmen (50-249 Mitarbeiter)
- bis zu 25 Prozent bei großen Unternehmen (mehr als 250 Mitarbeiter)

Förderfähig: **Personalkosten, Sachkosten** und **Gemeinkosten**

Aktueller Förderaufruf **bis zum 13. Oktober 2023**!

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Simon Schneider

Projektmanager
Materialtechnologien
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simon.schneider@htai.de

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Hessisches Ministerium für Wirtschaft, Energie, Verkehr und Wohnen

Projektträger:
Hessen Trade & Invest GmbH

TU DARMSTADT – ADVANCED THIN FILM TECHNOLOGY

Standnummer 16

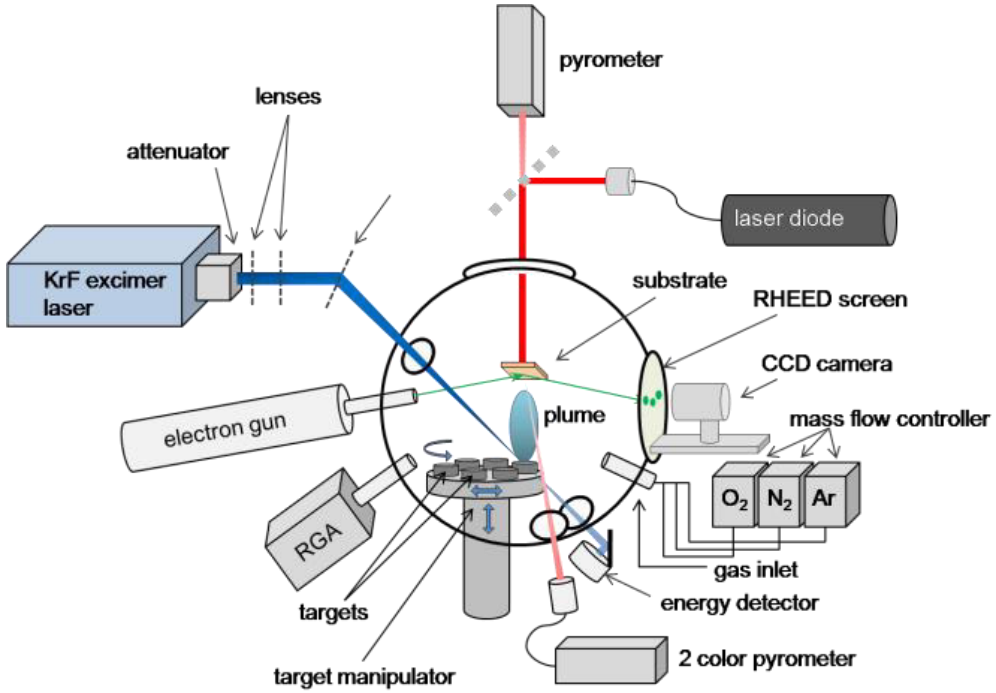


DÜNNE SCHICHTEN
(ADVANCED THIN FILM TECHNOLOGY)

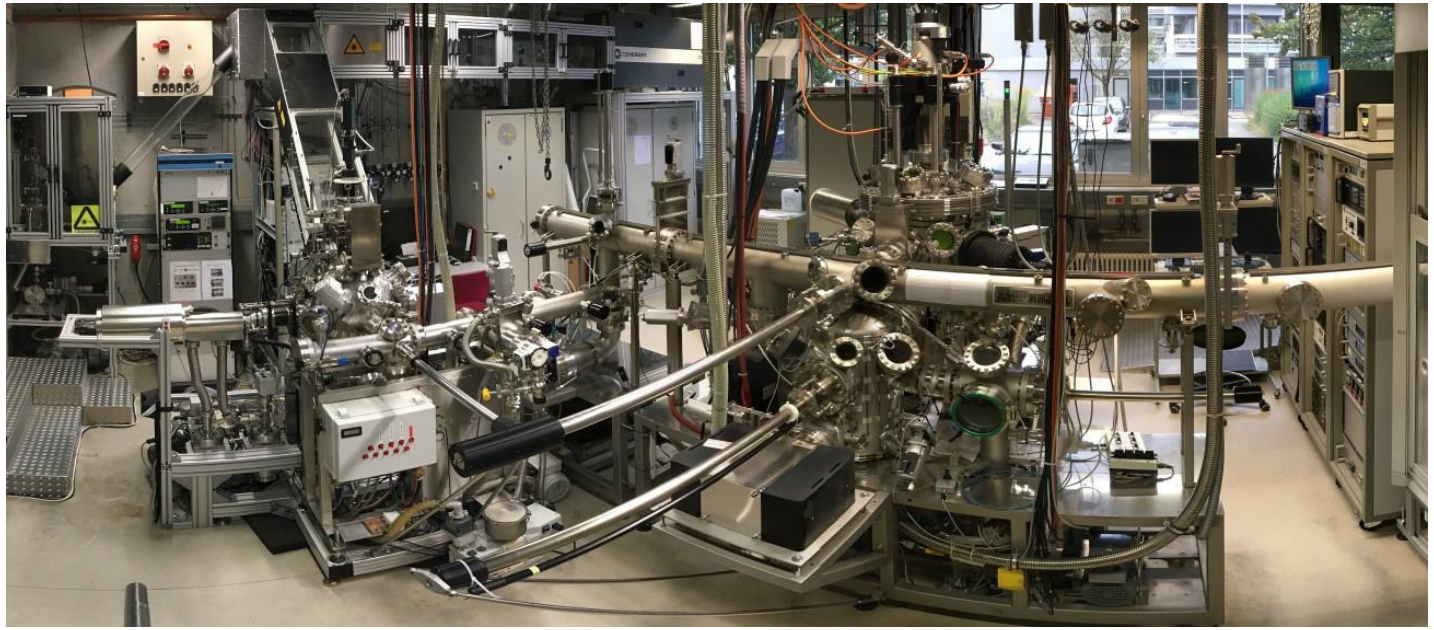
PROF. DR. LAMBERT ALFF

© Thomas Ott

TECHNISCHE UNIVERSITÄT DARMSTADT



Pulsed Laser Deposition (PLD)

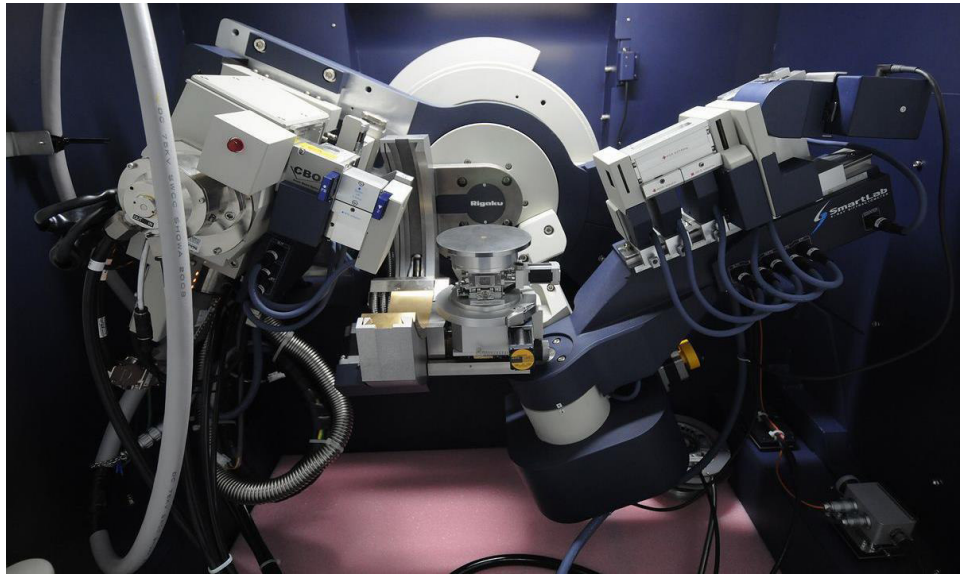


Cluster: PLD & Oxide-Molecular beam epitaxy (ADOMBE)

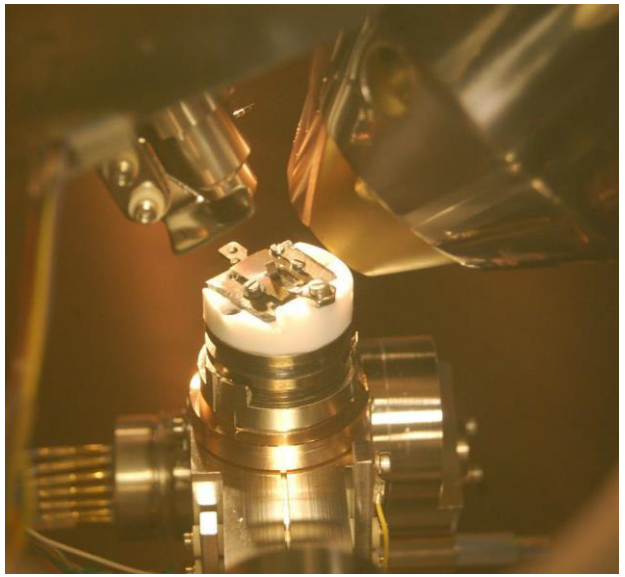


Several sputter units

All systems connected by vacuum transfer chamber

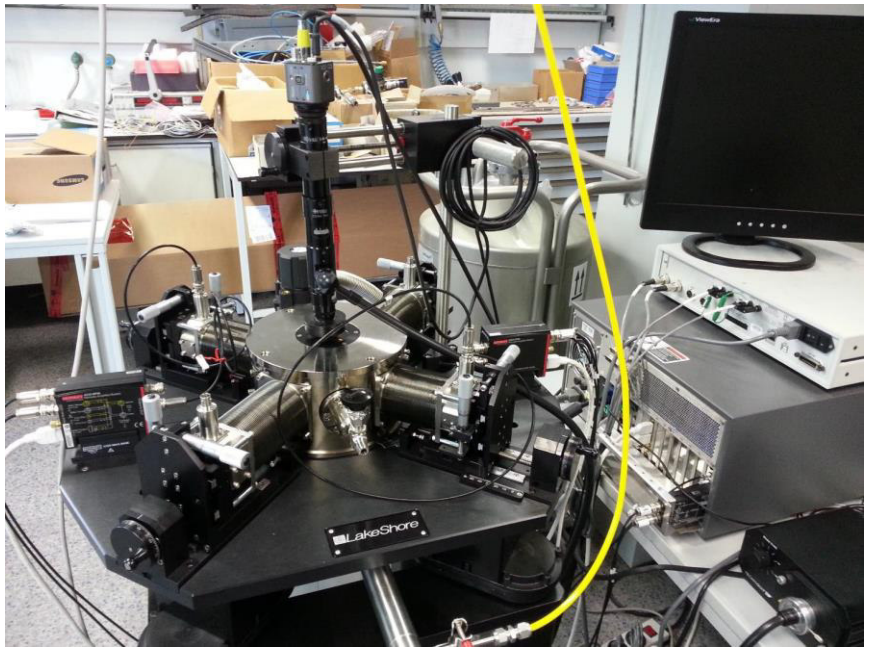


XRD (Rigaku & Bruker)



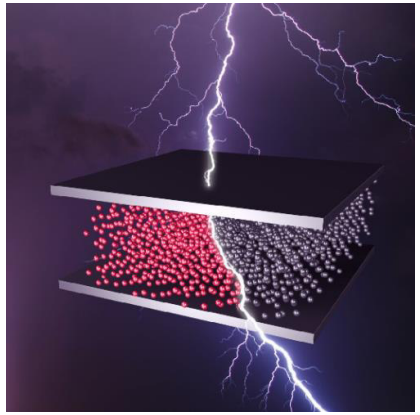
XPS (in situ)

SQUID (magnetic characterization)
Cryostats (16 T)
UV/Vis
PE-Loop tracer…



Electrical characterization

TECHNISCHE UNIVERSITÄT DARMSTADT



Electronic devices
(Memristoren for AI, rf devices)

StorAIge

STMicroelectronics

Fraunhofer

BMBF



Superconducting coatings:
Energy efficient accelerators

DFG Deutsche Forschungsgemeinschaft

Various projects

MERCK

infineon

For Mikro 2

BMBF

SFB/TRR 270 HoMMage

26 Fe Iron 55.845

Iron, upgraded!
CRC 1487

Resource efficient
magnetic materials

Industry
collaboration
by mutual





MATERIAL-
WISSENSCHAFT

TECHNISCHE
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DARMSTADT

SCHOTT AG

Standnummer 17



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Specialty glass

for more than 130 years

Our competence lies in the areas of specialty glass, glass-ceramics and other innovative materials.

The company’s founder Otto Schott is considered the founder of the specialty glass industry.

Since Otto Schott, innovations have always been a part of SCHOTT’s DNA. Therefore, we have 685 researchers and 17.200 employees worldwide sharing our passion.



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Where passion meets cutting-edge technology

Fire place



Photobioreactors



Telescope mirrors



Ultra thin glass
e.g. smartphone cover





Augmented Reality



Electronic packaging, e.g.TGV
wafers for MEMS devices



Light guide rods,
e.g. dental applications

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SCHOTT
glass made of ideas

Central R&D competence fields and competencies

Unique-Synergistic-Performing

MATERIAL DEVELOPMENT	MELTING*	HOT FORMING & PROCESSING*	LASER PROCESSING*	COATING & SURFACE MODIFICATION*
Specialty glass Glass ceramics Powders, pastes & inks Laser glass IR materials Polymer & Composites* Materials Informatics	Melting technology Melting Labs (GER, US)	Hot forming Hot processing	Cutting & structuring Decor & marking (Re)forming Polymer processing Additive Manufacturing	Functional & decorative coating Coating & printing materials Printing Liquid phase coating Gas phase coating Plasma modification

DATA SCIENCE

Data acquisition, Data analysis, Models for prediction and anomaly detection, Defect detection and classification

* Emerging technologies: new fields under evaluation

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Material Development & Advanced Processing

We develop a wide range of materials that address diverse properties and applications

Mechanical stability

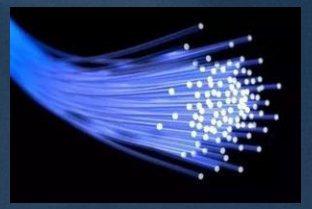
- Toughened cover glass
- Ultra-thin glass for foldables and satellites



Optical Brilliance

- Ultra-high refractive index glass for AR applications
- Low-attenuation glass fibers

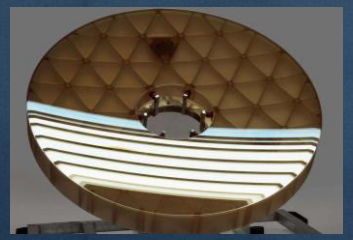


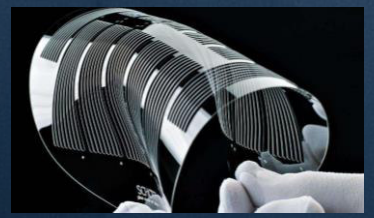


Geometrical precision

- Glass ceramics with negatively expanding crystals
- Zero-thermal-expansion materials for extreme conditions
- Laser processing

  e.g. ultra thin glass wafers





Next Gen Structuring – Flexinity ®

Functional Materials & Surfaces

- Solid Lithium-conductors
- Enabling safe, high-energy ASSBs (all-solid-state batteries)





EVERIC® care and smooth

- High performance coatings and surface modifications

  e.g. For pharmaceutical packaging

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Mission Zero Carbon

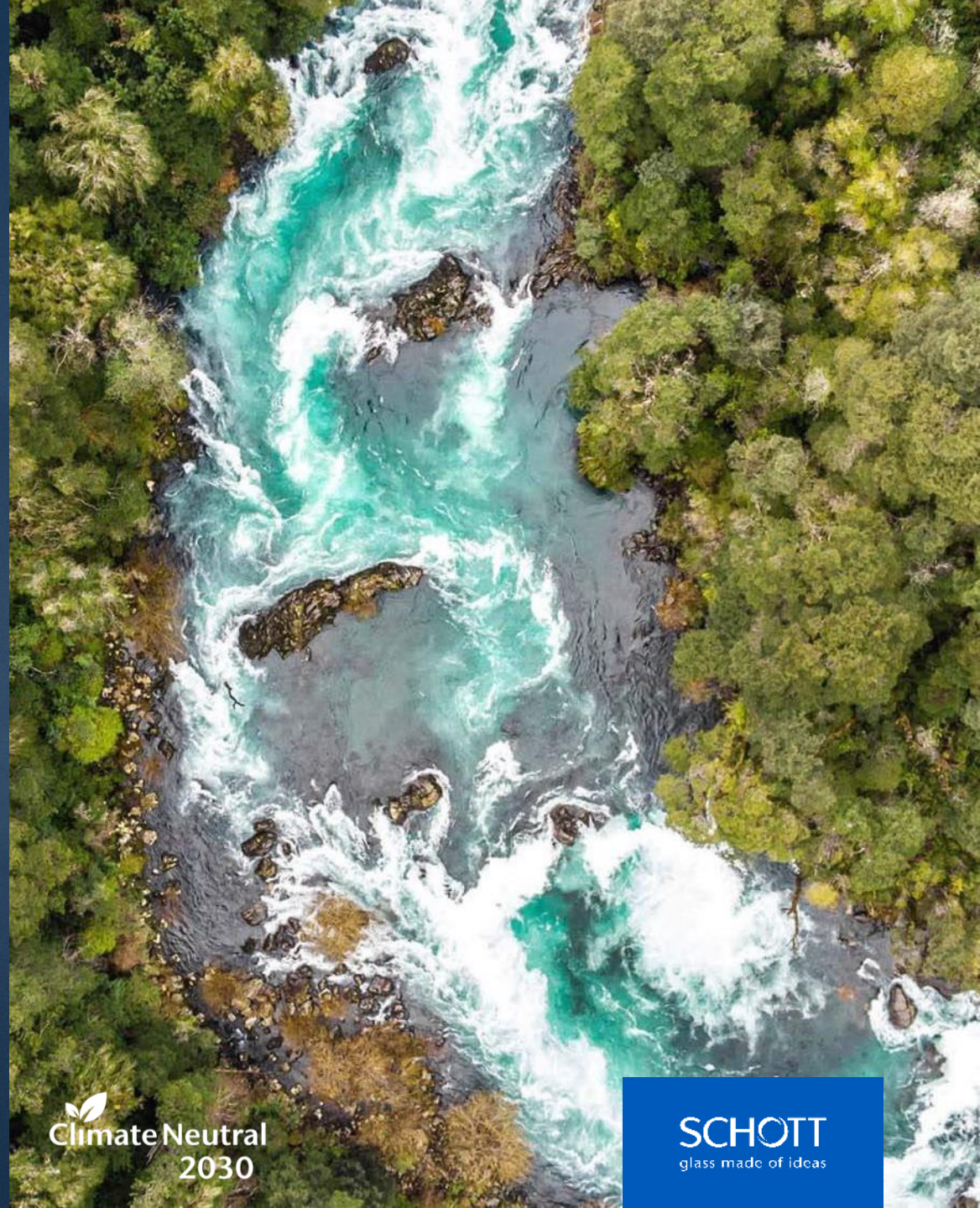
Commitment: Carbon Neutral 2030 in our production (Scope1 & Scope 2 GHG Protocol)

- Special glasses require high melting temperatures of up to 1.700 °C.
- Traditionally, melting tanks have been heated with fossil fuels, natural gas and heating oil or electricity
- Climate-relevant footprint amounted to 1 million tons CO_2e per year in 2019

Several ambitious R&D Projects



- New hot forming and melting technologies:
  H_2, plasma, microwave,
  full-electric melting



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Curious?
We are happy to answer questions and discuss at our booth

Thanks!



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Questions?



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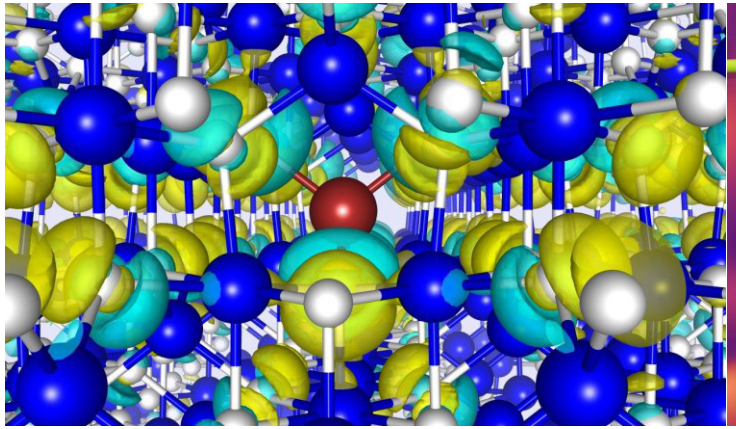
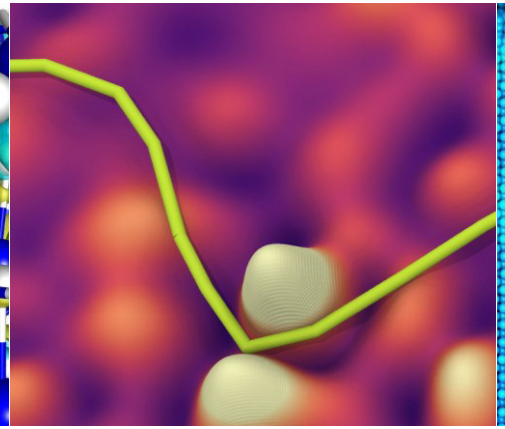
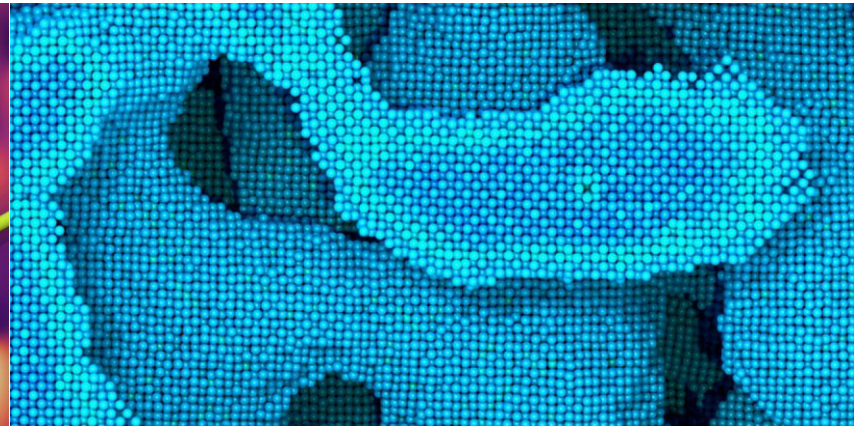
TECHNISCHE
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DARMSTADT

TU DARMSTADT – MATERIALMODELLIERUNG

Standnummer 18

Materials Modelling Division:
From computer simulations to experimental facts

TECHNISCHE UNIVERSITÄT DARMSTADT

Karsten Albe



DFG

Bundesministerium für Bildung und Forschung

Bundesministerium für Wirtschaft und Klimaschutz

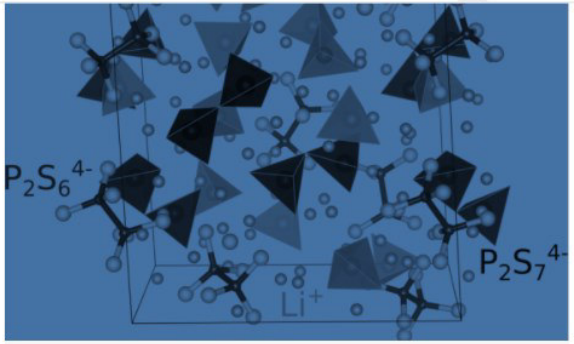
FLAIR

FEST BATT
Cluster of Competen.. for Solid-state Batteries

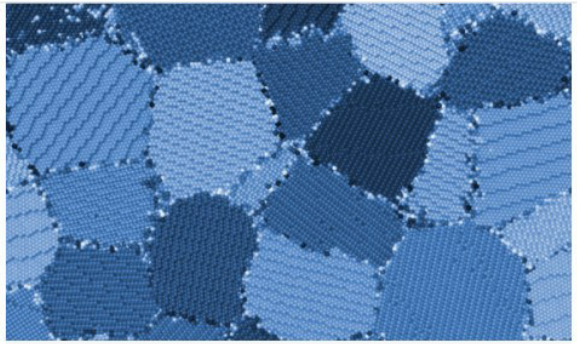
NHR4CES
NHR for Computational Engineering Science

Material Modellierung

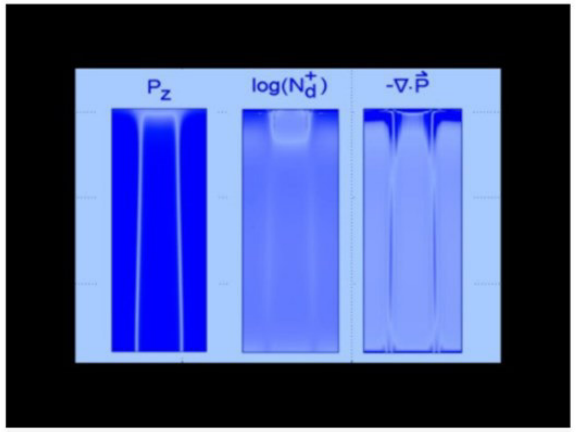
Materials Modeling Division: Topics



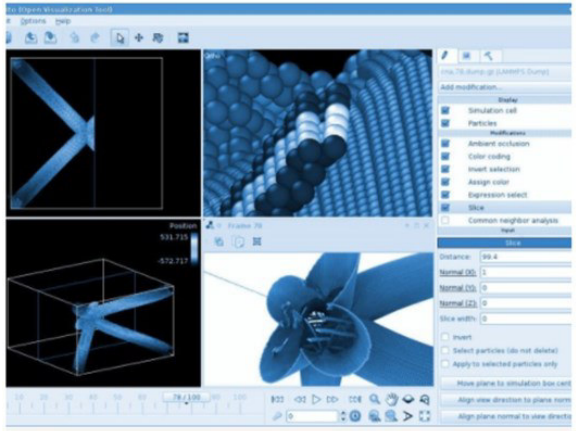
Energy Materials



Nanostructured Materials and Glasses



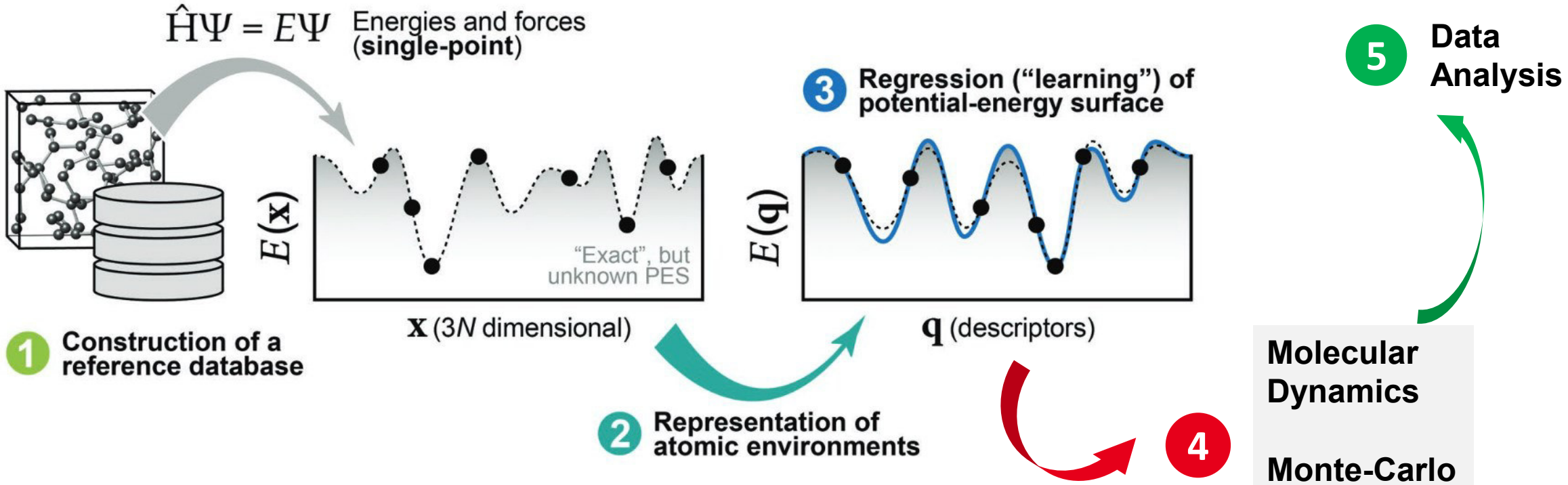
Functional Oxides



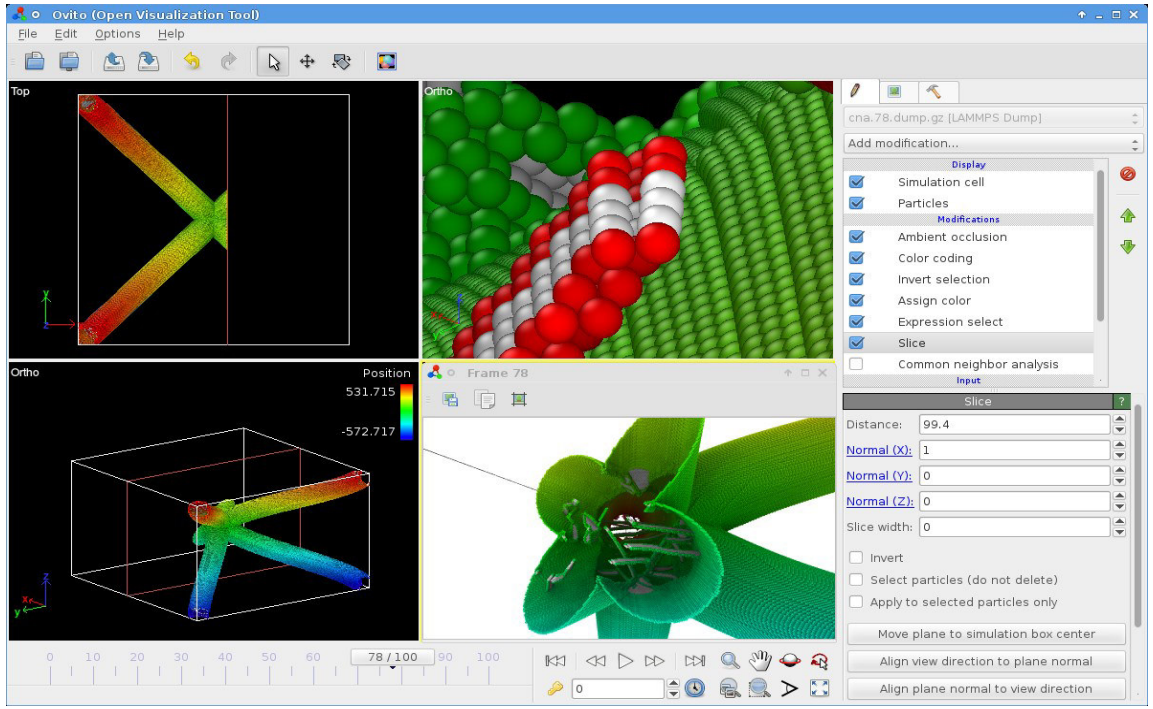
Methods and Software

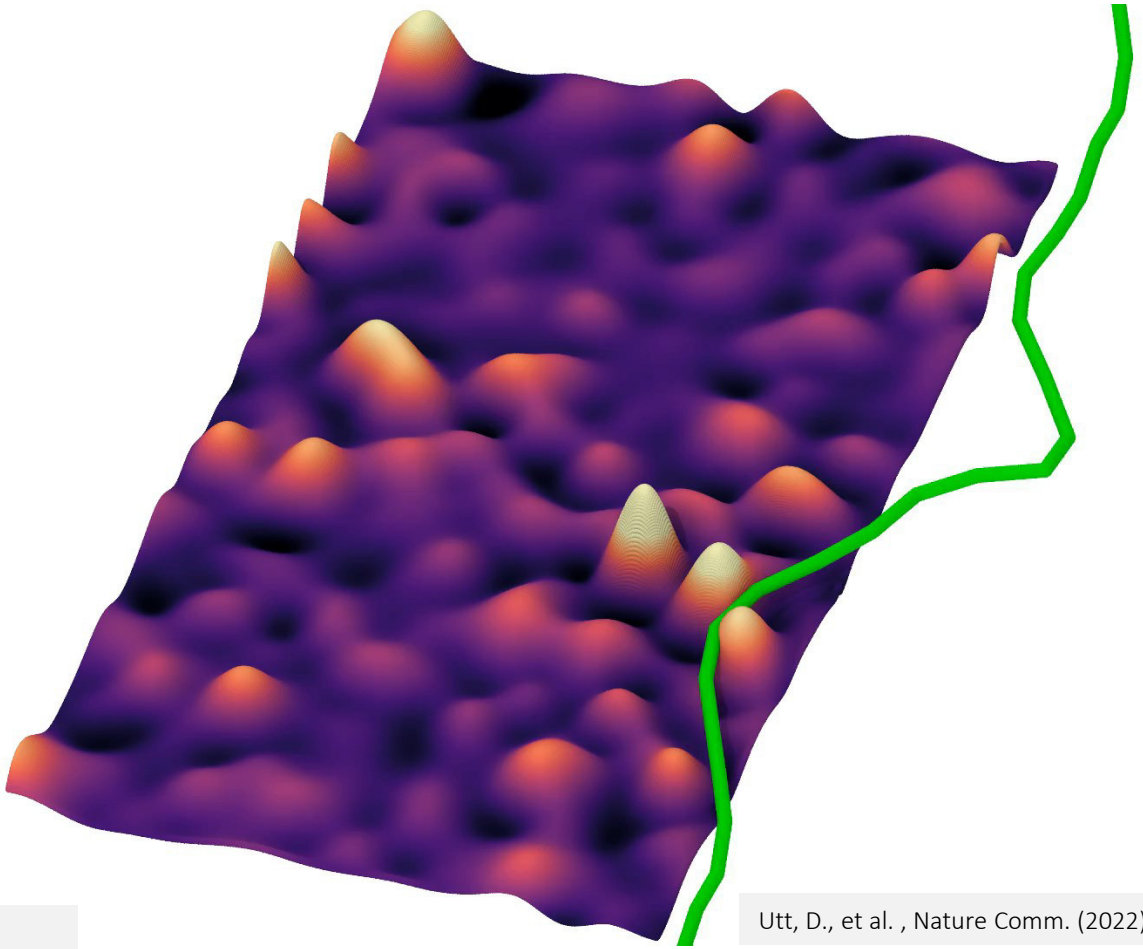


Methods: Atomistic Modelling



Methods: Dislocation pinning in high-entropy alloy



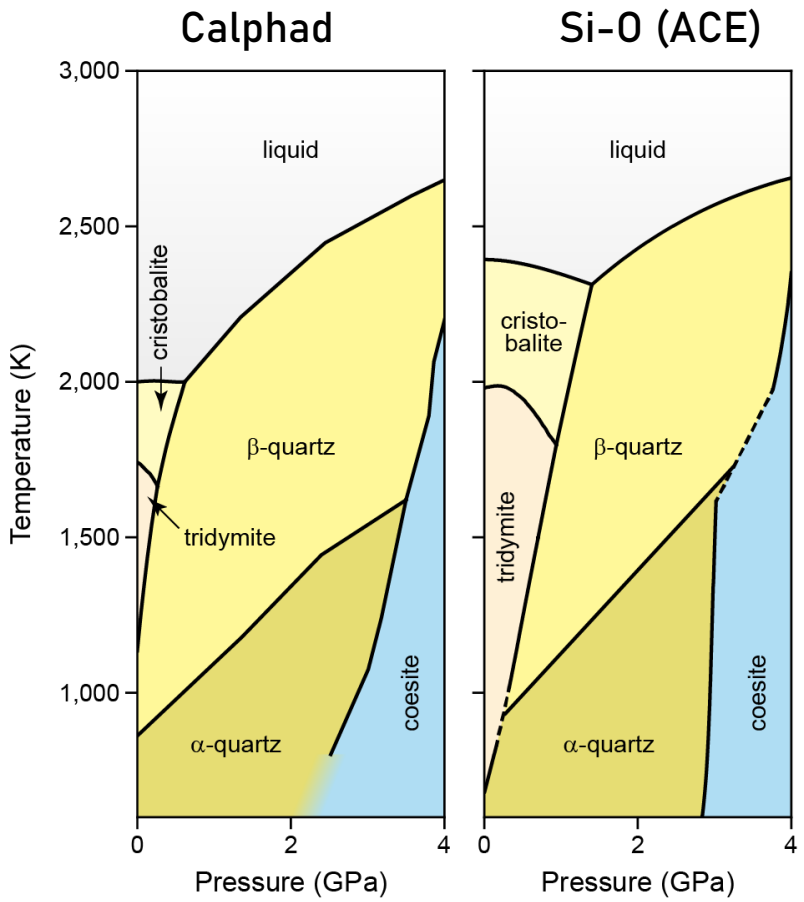


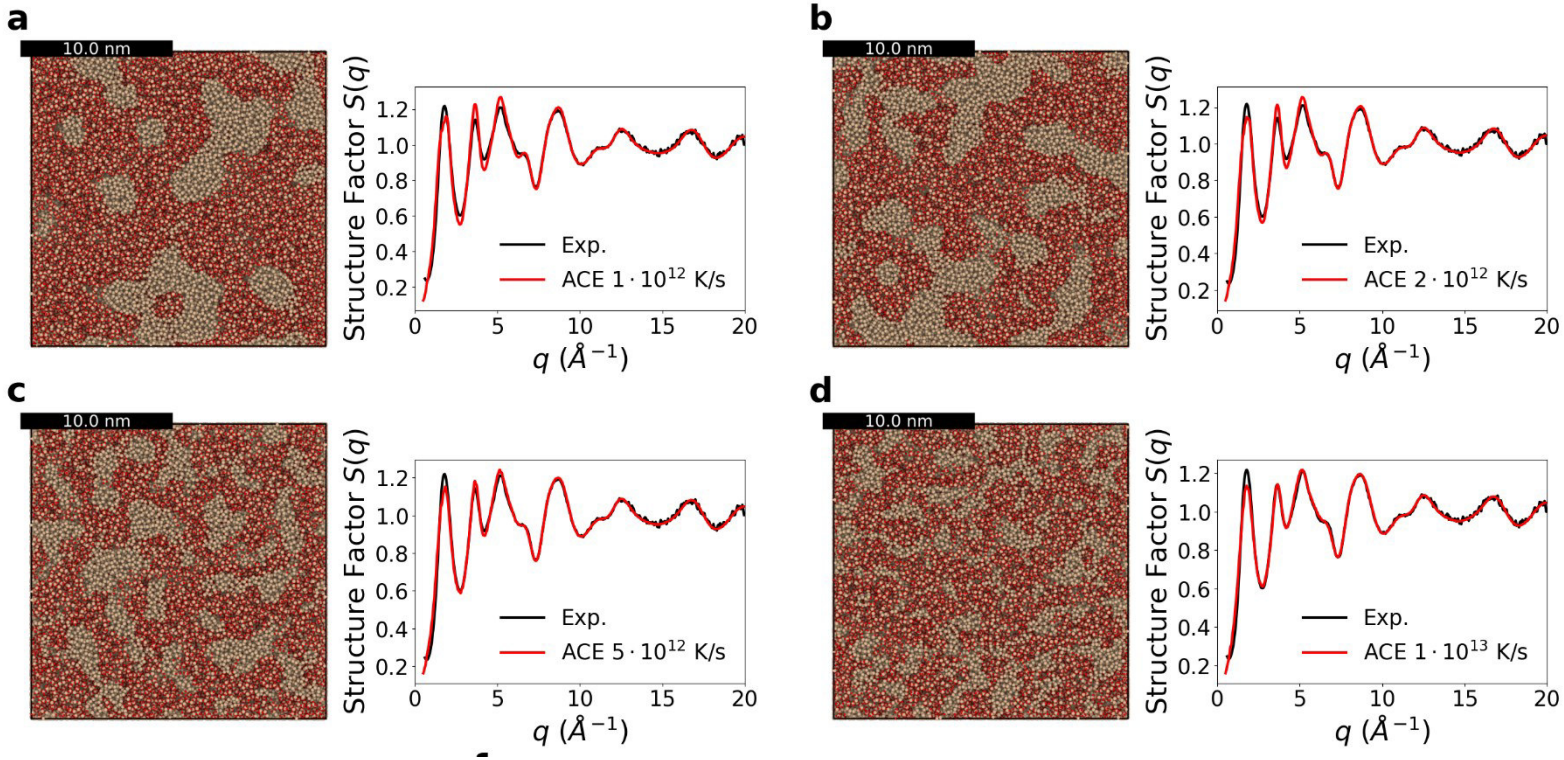
OVITO

Modelling Simul. Mater. Sci. Eng. 18 (2010), 015012

Utt, D., et al. , Nature Comm. (2022)

Nanostructured Materials and Glasses





Erhard et al., submitted, arXiv: 2309.03587

Energy Materials: Solid State Batteries

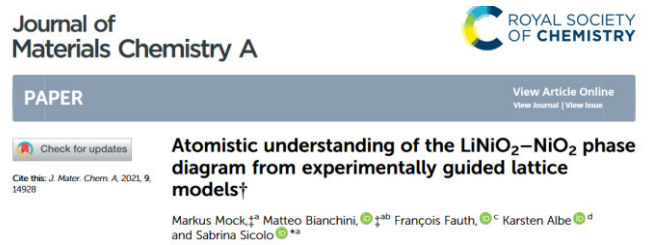
- **Properties of solid electrolytes**
- Enabling **Li metal anodes**
- Degradation of **cathode active materials**


CHEMISTRY OF MATERIALS

pubs.acs.org/cm Article

And Yet It Moves: $LiNiO_2$, a Dynamic Jahn–Teller System

Sabrina Sicolo,* Markus Mock, Matteo Bianchini, and Karsten Albe


Journal of Materials Chemistry A

ROYAL SOCIETY OF CHEMISTRY

PAPER View Article Online

Check for updates

Cite this: J. Mater. Chem. A, 2021, 9, 14928

Atomistic understanding of the $LiNiO_2$–NiO_2 phase diagram from experimentally guided lattice models†

Markus Mock,‡[a] Matteo Bianchini,‡[ab] François Fauth,[c] Karsten Albe[d] and Sabrina Sicolo*[a]


Solid State Ionics 363 (2021) 115604

Contents lists available at ScienceDirect

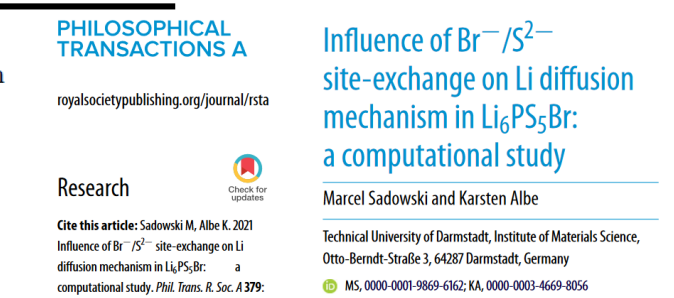
Solid State Ionics

journal homepage: www.elsevier.com/locate/ssi

From ionic to superionic conductivity: The influence of cation order on sodium diffusion in $Na_3Zr_2Si_2PO_{12}$

L. Haarmann*, K. Albe

Technische Universität Darmstadt, Institut für Materialwissenschaft, Fachgebiet Materialmodellierung, Otto-Berndt-Str. 3, Darmstadt D-64287, Germany


PHILOSOPHICAL TRANSACTIONS A

royalsocietypublishing.org/journal/rsta

Research

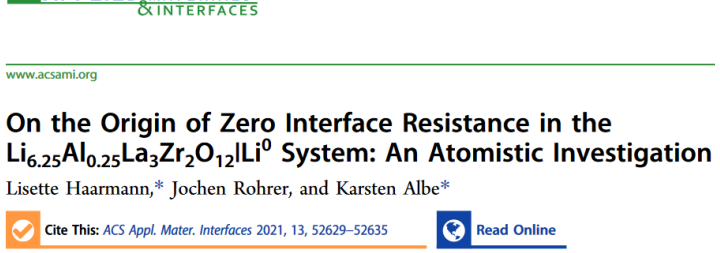
Cite this article: Sadowski M, Albe K. 2021 Influence of Br^-/S^{2-} site-exchange on Li diffusion mechanism in Li_6PS_5Br: a computational study. *Phil. Trans. R. Soc. A* 379:

Influence of Br^-/S^{2-} site-exchange on Li diffusion mechanism in Li_6PS_5Br: a computational study

Marcel Sadowski and Karsten Albe

Technical University of Darmstadt, Institute of Materials Science, Otto-Berndt-Straße 3, 64287 Darmstadt, Germany

MS, 0000-0001-9869-6162; KA, 0000-0003-4669-8056


ACS APPLIED MATERIALS & INTERFACES

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On the Origin of Zero Interface Resistance in the $Li_{6.25}Al_{0.25}La_3Zr_2O_{12}|Li^0$ System: An Atomistic Investigation

Lisette Haarmann,* Jochen Rohrer, and Karsten Albe*

Cite This: ACS Appl. Mater. Interfaces 2021, 13, 52629–52635

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FULL PAPER

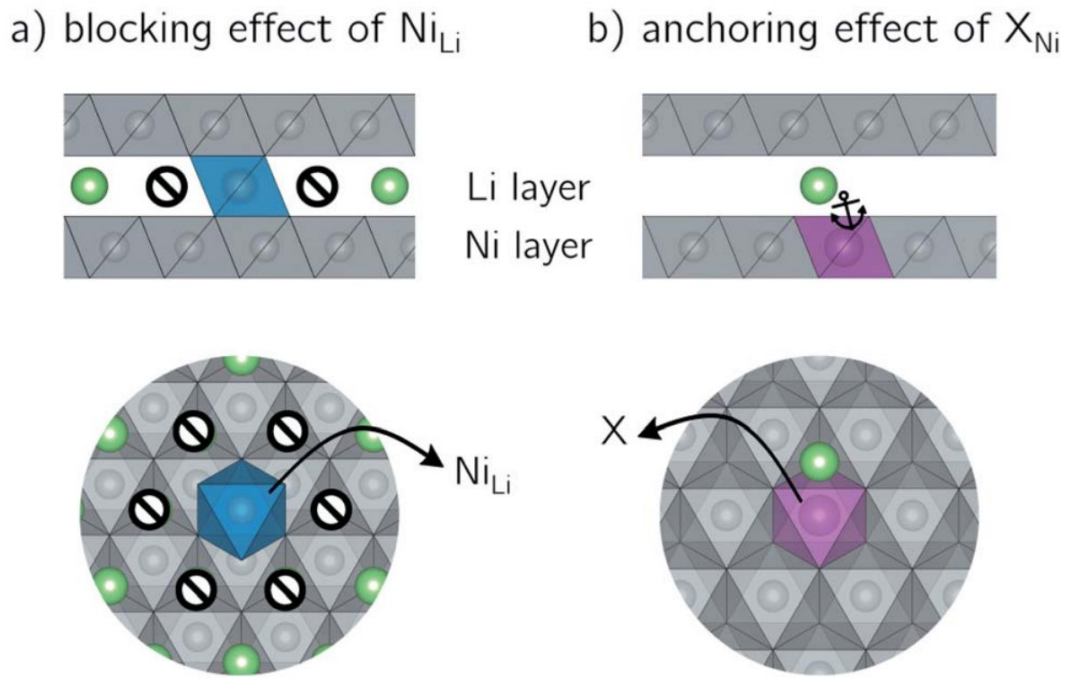
ADVANCED ENERGY MATERIALS

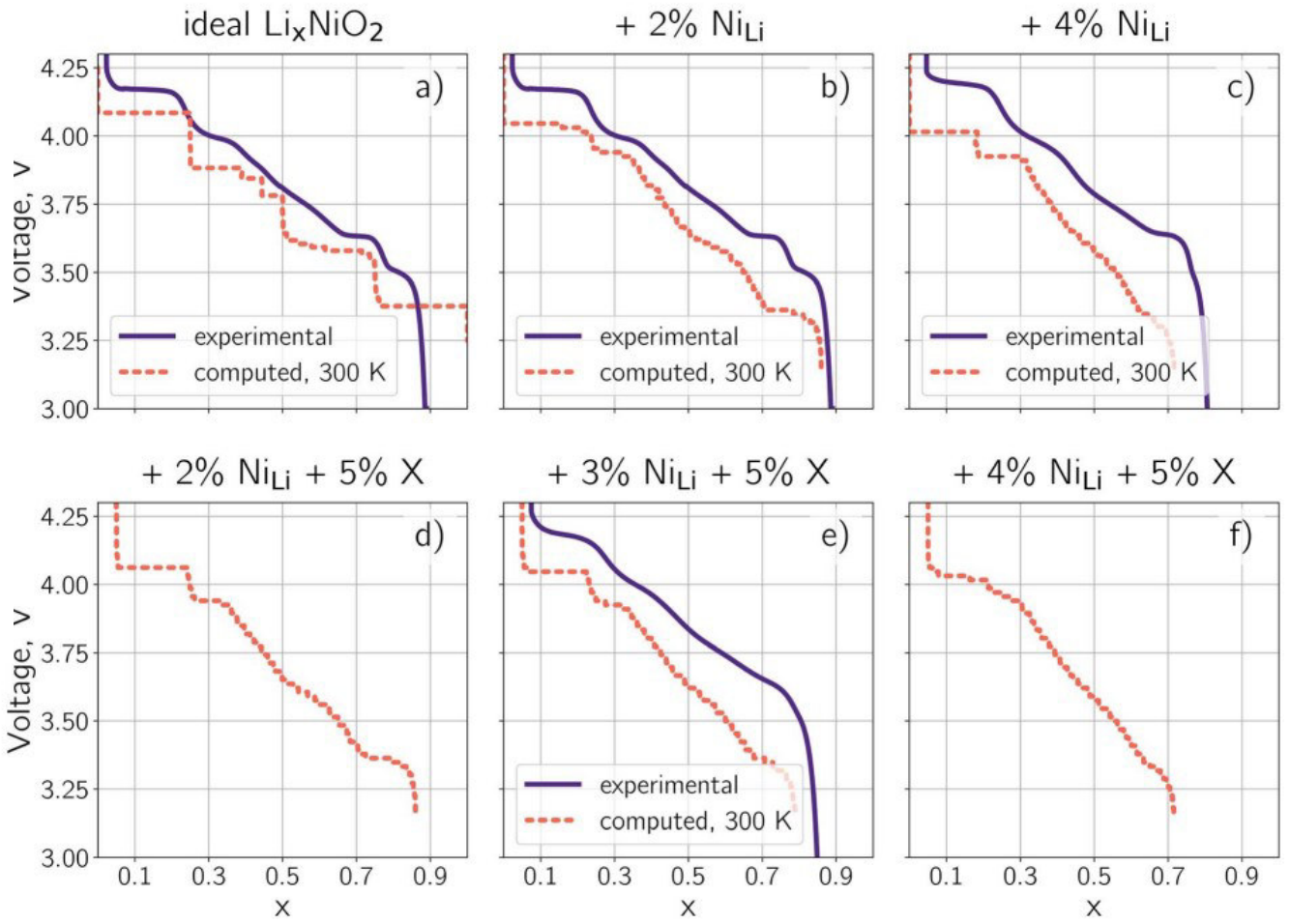
www.advenergymat.de

Engineering the Site-Disorder and Lithium Distribution in the Lithium Superionic Argyrodite Li_6PS_5Br

Ajay Gautam, Marcel Sadowski, Michael Ghidiu, Nicolò Minafra, Anatoliy Senyshyn, Karsten Albe, and Wolfgang G. Zeier**

Energy Materials: Defects matter





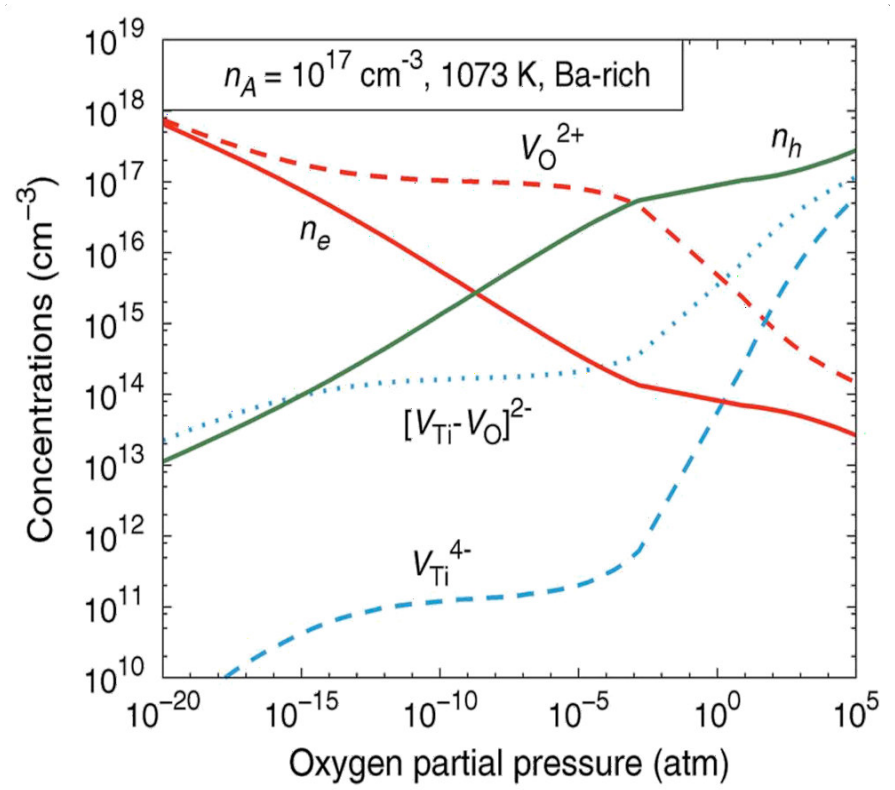
Disruption of ordering by redox inactive dopants !

M. Mock et al., J. Mater. Chem. A, 2021, 9, 14928

Functional Oxides: ab-initio Defect Thermodynamics

Defect formation energy	$\Delta H = \Delta H_{D,q}(\mu, E_F)$
Defect concentration	$c_D \approx N_{site} \times \exp(-\Delta H/kT)$
Electron/hole density	$c_e = \int f_{FD}(E-E_F)\, g(E)\, dE$
Charge neutrality	$-c_e + c_h + \Sigma\,[q \cdot c(D^q)] = 0$
Self-consistent solution	$\Delta H(E_F) \longrightarrow c_D(\Delta H) \longrightarrow E_F$
pO_2 dependence of μ_O	$\Delta\mu_O(T,P_0) = \frac{1}{2}[H_0+\Delta H(T)] - \frac{1}{2}T\cdot[S_0+\Delta S(T)]$
(ideal gas)	$\Delta\mu_O(T,P) = \Delta\mu_O(T,P_0) + \frac{1}{2}kT\ln(P/P_0)$

High conc.	Account for competition of defects and host atoms for N_{site} Association/dissociation of ***defect-clusters*** (law of mass action)
Direct	Given $\Delta H(\mu)$, find concentrations c_D
Inverse	Given a target concentration, find ΔH (i.e., find μ)



Erhart, Albe, JOURNAL OF APPLIED PHYSICS 104, 044315, 2008

Materials Modeling Division@TU Darmstadt



"Our ambition is to explain or predict properties of defects in materials by computer simulations based on solid-state physics, statistical and materials mechanics.

MATERIAL-
WISSENSCHAFT

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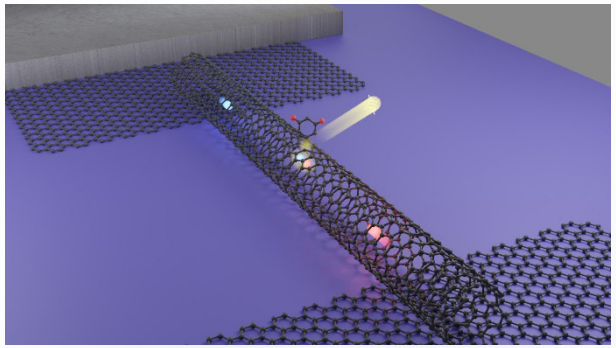
TU DARMSTADT & KIT – MOLEKULARE NANOSTRUKTUREN

Standnummer 19

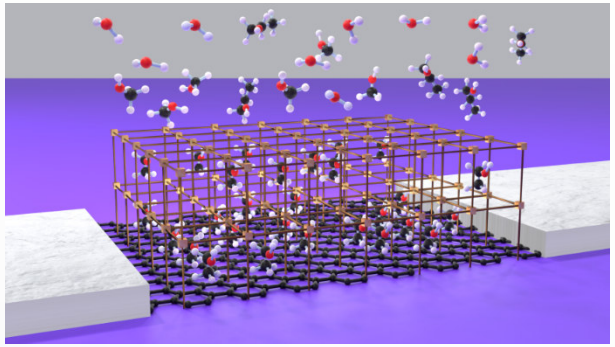
Division Molecular Nanostructures – Research Topics

TECHNISCHE UNIVERSITÄT DARMSTADT

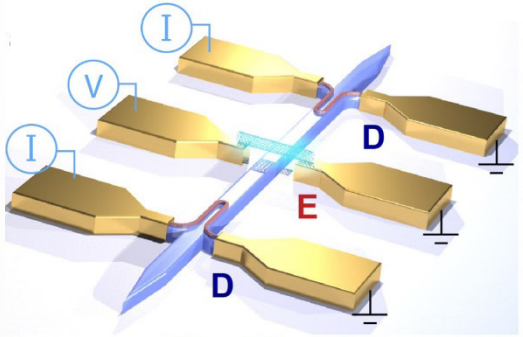
Focus on nanoscale light emission, infrared photodetection, high-mobility transistors, superconducting currents and molecular sensors.



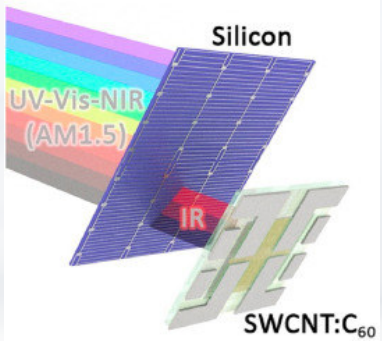
Nat. Mater. 2018, ACS Nano 2022



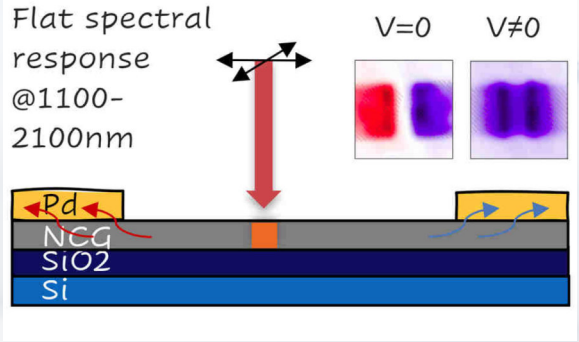
Adv. Mat. 2021, Adv. Electron. Mater. 2023



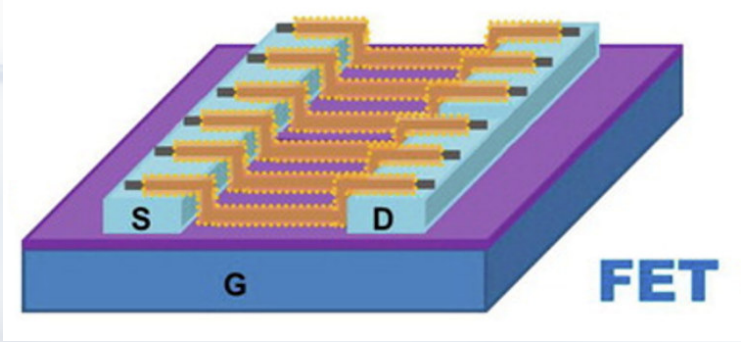
Nat. Photonic. 2016, Nat. Commun 2023



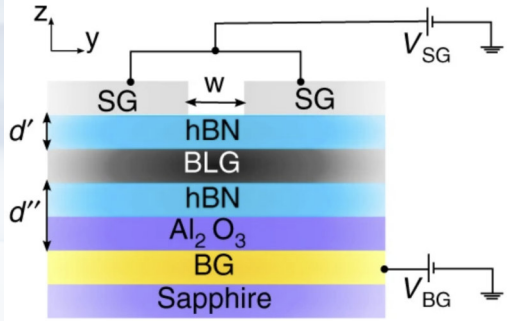
Carbon 2021, Small 2023



ACS Appl. Mater. Interfaces 2022



ACS Nano 2016, Comm. Phys. 2021



Nat. Commun 2018, Phys. Rev. Lett. 2021

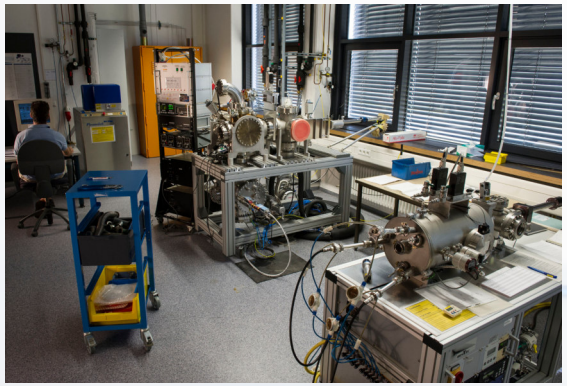
Division Molecular Nanostructures – Methods & Materials

TECHNISCHE UNIVERSITÄT DARMSTADT

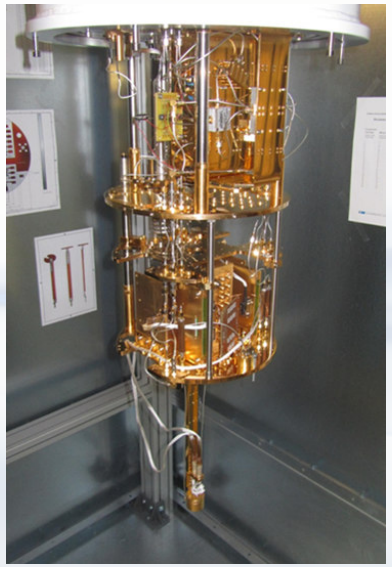
Synthesis, purification, nanofabrication, device integration and characterization @ KIT and TUDa

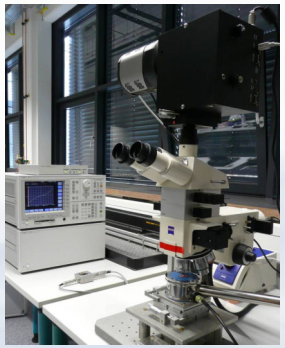
Low-dimensional materials synthesis, e-beam lithography, reactive ion etching, sputtering, thermal evaporation, atomic-layer deposition, dielectrophoresis, stacking, liquid-phase processing and sorting, packaging

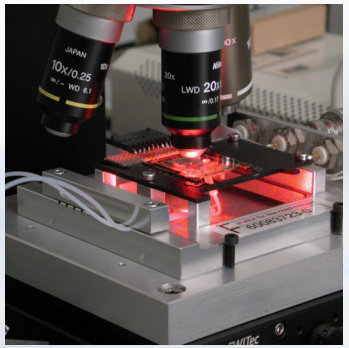




Visible-nearInfrared electroluminescence and photocurrent spectroscopy and imaging, single-photon detection, Raman imaging, semiconductor parameter analysis, low-temperature and milliKelvin experiments







Posters

TECHNISCHE UNIVERSITÄT DARMSTADT

Sensitive Detection of Ethanol Molecules with Low-Power Metal-Organic Framework Functionalized Carbon Nanotube Transistors

Karlsruhe Institute of Technology

Sandeep Kumar,[a] Simone Dehm,[a] Laura Wieland, [a,c] Abhinav Chandresh,[d] Lars Heinke,[d] Benjamin S. Flavel,[a] and Ralph Krupke[a,b,c]

[a]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany
[b]Institute of Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany
[c]Institute of Materials Science, Technische Universität Darmstadt, 64827 Darmstadt, Germany
[d]Institute of Functional Interfaces, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

TECHNISCHE UNIVERSITÄT DARMSTADT



Dr. Kumar

Enhanced Broadband Photodetection with Geometry and Interface Engineered Nanocrystalline Graphite

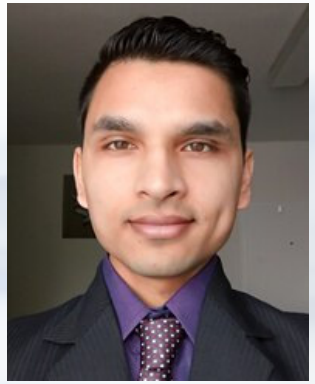
Karlsruhe Institute of Technology

Devang Parmar,[a,b,c] Simone Dehm,[b] Naga Anirudh Peyyety,[a,c] Sandeep Kumar,[a] and Ralph Krupke[a,b,c]

[a]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany
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TECHNISCHE UNIVERSITÄT DARMSTADT

DFG Deutsche Forschungsgemeinschaft



M.Sc. Parmar

- Electroluminescence from single-walled carbon nanotubes with quantum defects

MATERIAL-
WISSENSCHAFT

TECHNISCHE
UNIVERSITÄT
DARMSTADT

TU DARMSTADT– THEORIE MAGNETISCHER MATERIALIEN

Standnummer 20

14.11.2023



INVERSE DESIGN OF FUNCTIONAL MATERIALS

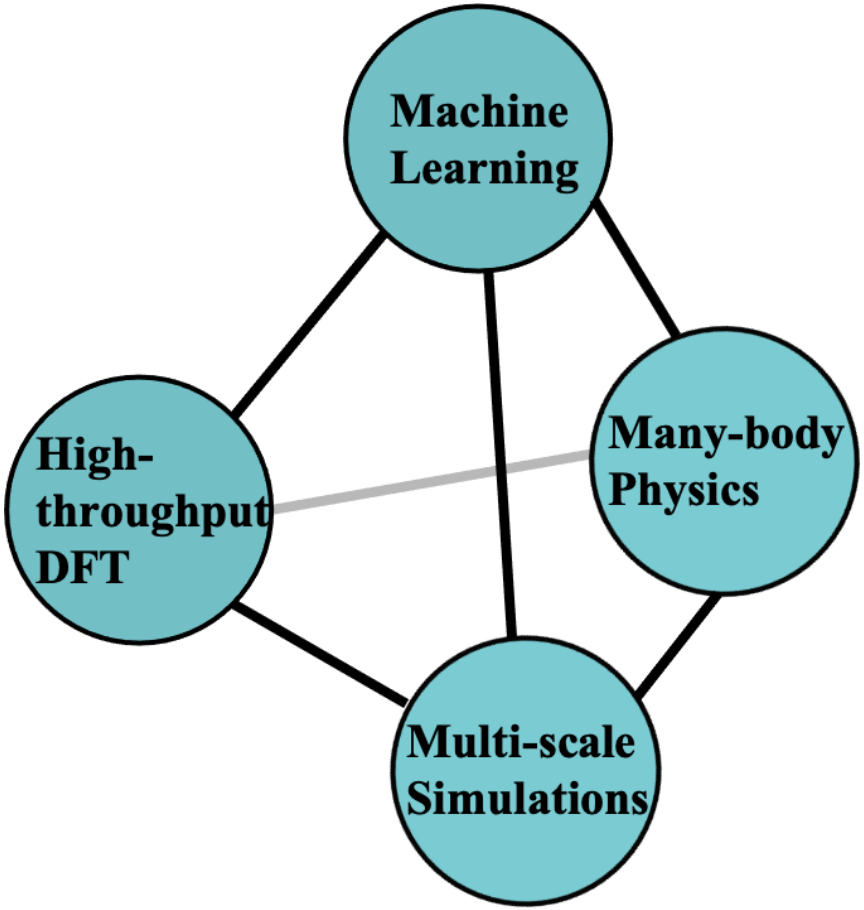
hongbin.zhang@tu-darmstadt.de

@hongbin_zhang

www.linkedin.com/in/zhang-tuda

OVERVIEW OF RESEARCH IN MY GROUP

TECHNISCHE UNIVERSITÄT DARMSTADT



OVERVIEW OF RESEARCH IN MY GROUP

TECHNISCHE UNIVERSITÄT DARMSTADT

Permanent magnets
- Heusler w/ interstitials, ActaM, 186, 355 (20')
- Cu_3Au w/ interstitials, PRR 2, 023134 (20')
- MAB phases, JMCA 9, 8805 (21')

Magnetocaloric materials
- MM'X, Adv. Sci. 2206772 (23')
- all-d-metal Heusler (to be submitted)
- Co-based Heusler (in preparation)

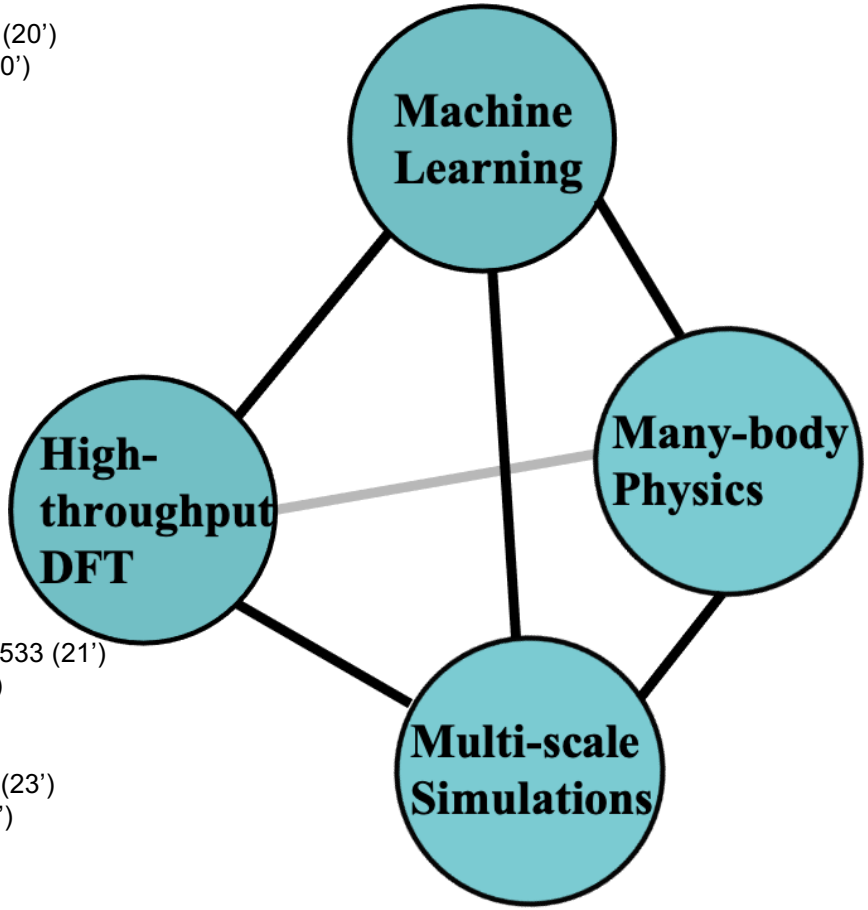
Topological insulators & transports
- automated WF, JPCL **9**, 6224 (18')
- spin gapless SC, PRM **3**, 024410 (19')
- TM-based FMs, JPD **55**, 074003 (21')
- SHC in Heusler, NJP **24**, 053027 (22')
- half-APV, Acta **242**, 118474 (23')
- all-d-metal Heusler, AFM 2214967 (23')

Polarizable Materials
- AFE NN-SS, Chem. Mat. 33, 266 (20')
- KNN, Nat. Commun. 13, 3434 (22')
- ABC, Mat. Tod. Phys. 32, 100998 (23')

Thermal conductivity + thermoelectrics
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- $EuTiO_3$, Mat. Tod. Phys. 34, 101059 (23')

Photovoltaic materials
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Catalysts
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TECHNISCHE UNIVERSITÄT DARMSTADT

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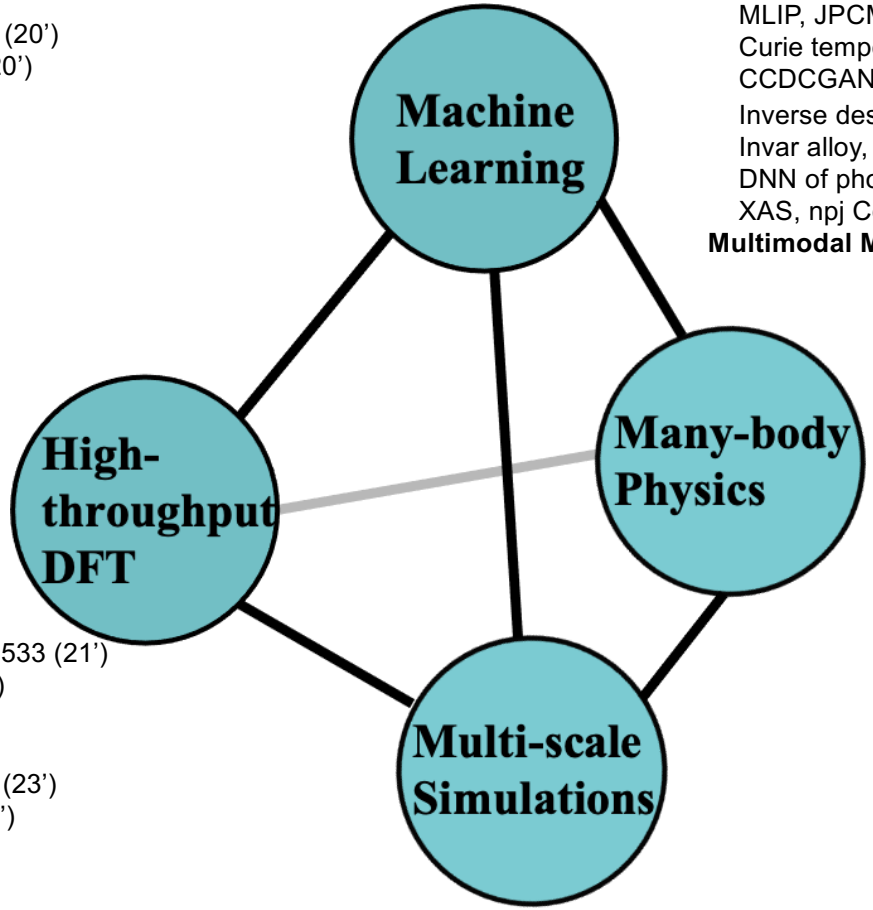
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Inverse design
- MLIP, JPCM 33, 105903 (20')
- Curie temperature of FM, MRL 9, 169 (21')
- CCDCGAN, npj Comput. Mat. 7, 66 (21')
- Inverse design, ActaM, 231, 117898 (22')
- Invar alloy, Science 378, 78 (22')
- DNN of phonons, npj Comput. Mat. 9, 20 (23')
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Multimodal ML of spectroscopies

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TECHNISCHE UNIVERSITÄT DARMSTADT

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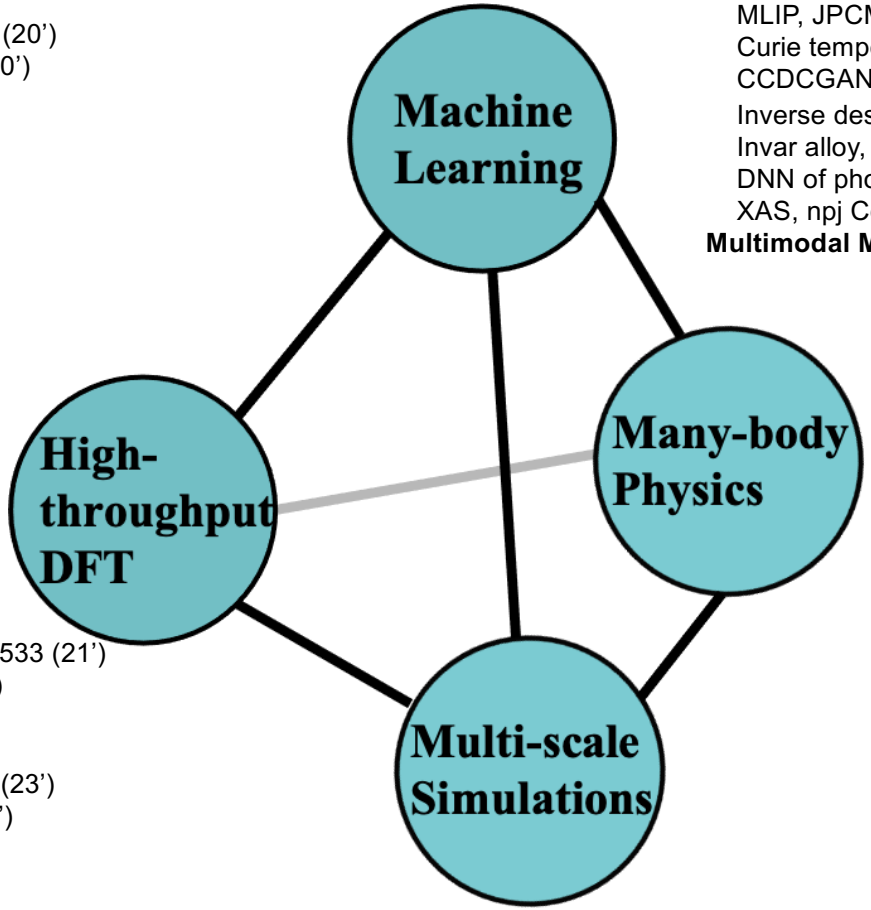
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- $SrMoO_3$, JAP 119, 055302 (16')
- $RE_2Ir_2O_7$, PRL 118, 206404 (17')
- Distorted $SrVO_3$, PRM 3, 115001 (19')
- U in 2D materials, Nano. Adv. 2, 495 (20')
- $SmCo_5$ + H, Nat. Commun. 11, 4849 (20')
- DFT+DMFT of $CeCo_5$, PRB 106, 224411 (22')
- $SrV_{1-x}Mo_xO_3$, Adv. Mat. 35, 2206605 (23')

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TECHNISCHE UNIVERSITÄT DARMSTADT

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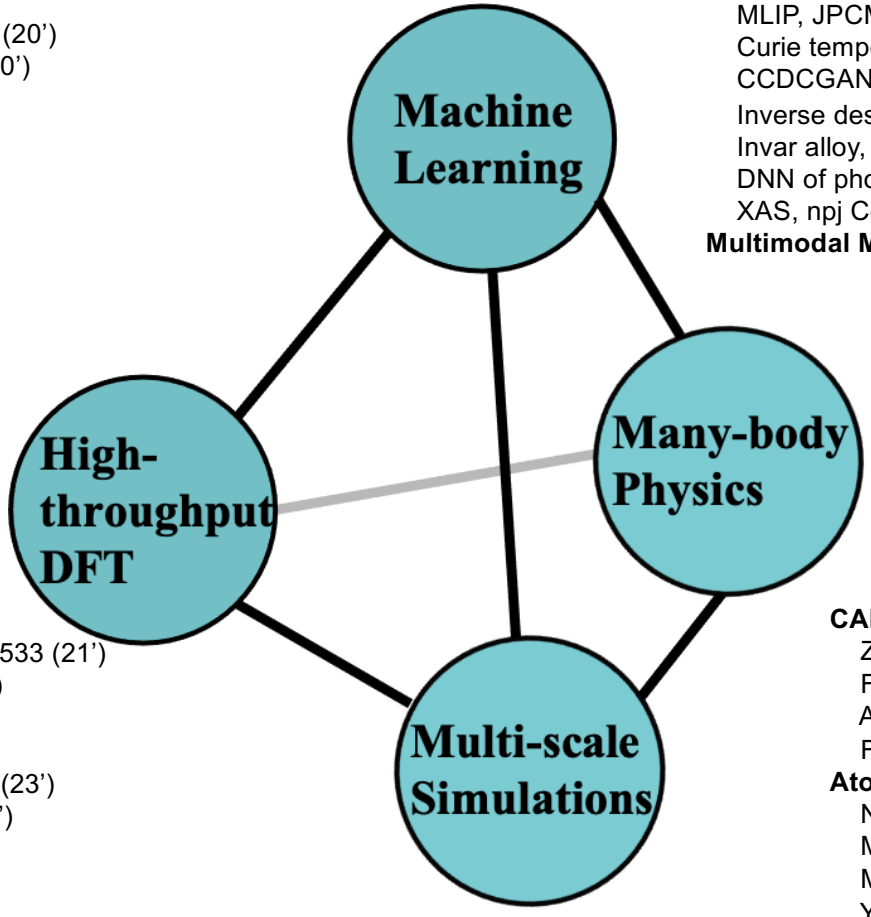
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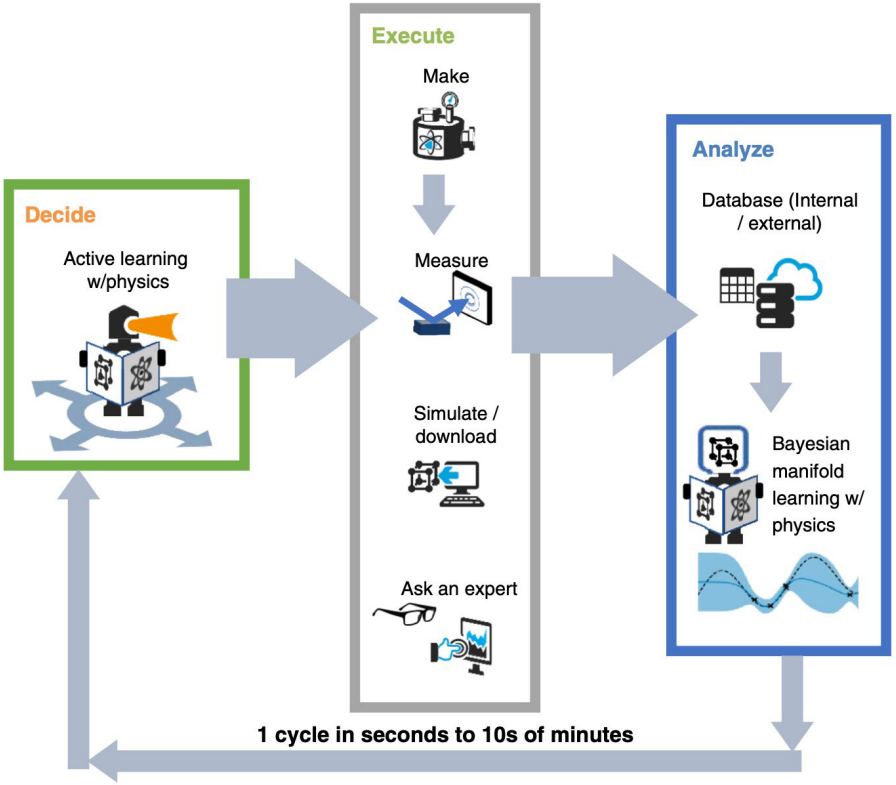
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- DFT+DMFT of $CeCo_5$, PRB 106, 224411 (22')
- $SrV_{1-x}Mo_xO_3$, Adv. Mat. 35, 2206605 (23')

CALPHAD
- Zr-Ti, CALPHAD 64, 213 (19')
- Fe-Y, J. Pha. Equil. Diff. 42, 348 (21')
- Au-In, J. Pha. Equil. Diff. 42, 479 (21')
- Fe-Sn, npj Comput. Mat. 8, 248 (22')

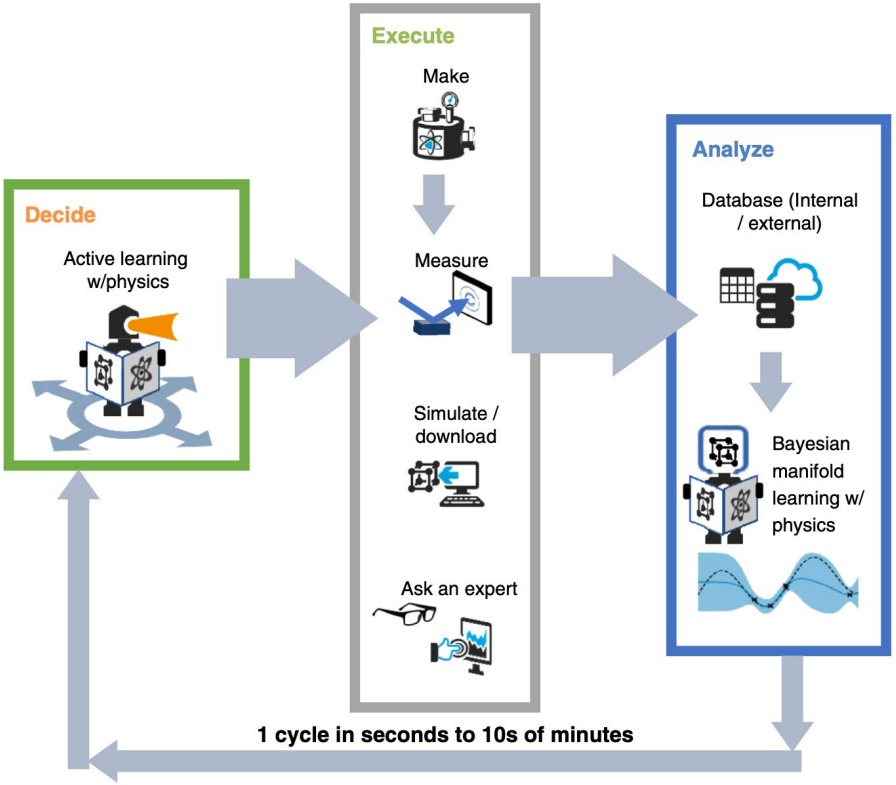
Atomistic spin dynamics
- Nd-Fe-B, Phys. Rev. Appl. 8, 014011 (17')
- MnBi/FeCo, PRB 98, 174440 (18')
- MnGa/FeCo, Phys. Rev. Appl. 11, 054078 (19')
- Y-Co, PRB 102, 014435 (20')
- Co/Pt3, Iscience 25, 104039 (22')
- $Nd_6Fe_{13}Cu$, APL 122, 242402 (23')

CLOSED-LOOP ADAPTIVE DESIGN

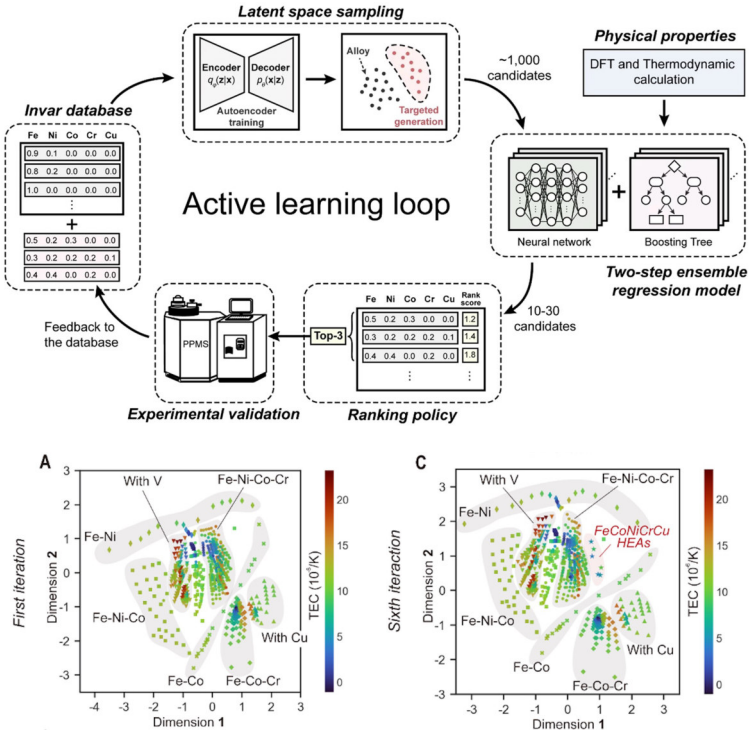


Closed-loop autonomous material exploration and optimization → industrial decision making

CLOSED-LOOP ADAPTIVE DESIGN



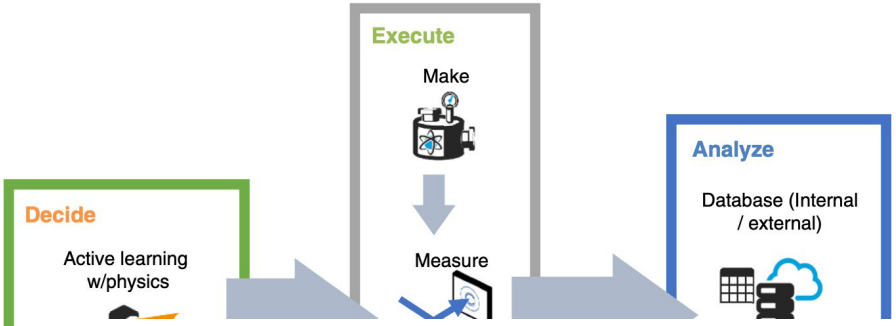
Closed-loop autonomous material exploration and optimization → industrial decision making

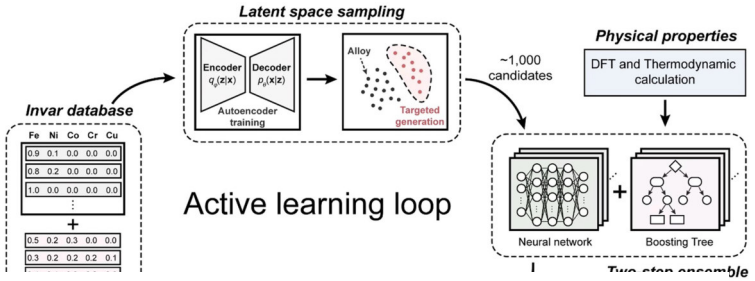


Closed-loop design of high-entropy Invar alloys

Z. Rao, et al., Science **378**, 78 (2022)

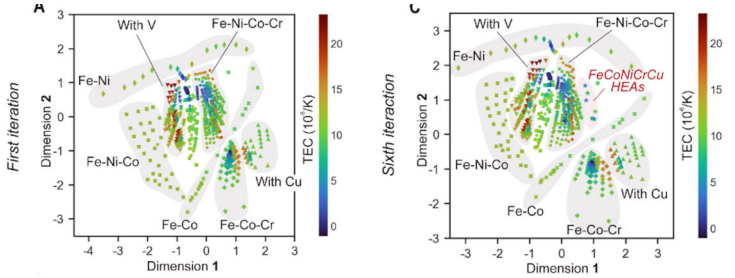
CLOSED-LOOP ADAPTIVE DESIGN





Transferprojekt T03 „Adaptives Design von Ni-Mn-Ga-X Heusler-Legierungen für die Anwendung als magnetische Formgedächtnislegierung im Hochtemperatur-bereich“ (Zhang)

Closed-loop autonomous material exploration and optimization → industrial decision making



Closed-loop design of high-entropy Invar alloys

Z. Rao, et al., Science **378**, 78 (2022)

MATERIAL-
WISSENSCHAFT

TECHNISCHE
UNIVERSITÄT
DARMSTADT

TU DARMSTADT– MECHANIK FUNTIONALER MATERIALIEN

Standnummer 21

17.11.2023

Topics of MFM group – Bai-Xiang Xu

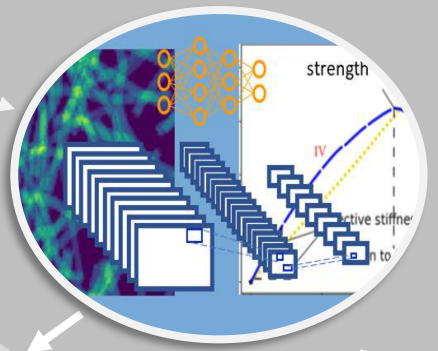


Advanced Processing

- Heat
- Sintering, solidification
- Melt flow dynamics
- Thermomechanics

Yang, et al. npj Comp. Mat., 2023
Yang, et al. Scripta Materialia 2020

Projects: TRR270, SPP2256, SPP2122, SFB1548
MOOSE App: **NIsoS**



Data-Driven Research

- Machine Learning
- Microstructure characterization
- Inverse Design

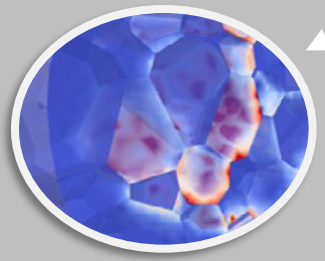
Lin et al. Materials & Design 2021
Lin et al. npj Comp. Mat. 2022

Projects: NHR4CES, GRK2561, PAK962

Process-**Microstructure**-Property
Multi-physics Mechanisms

Theory & Model
- Phase-field theory
- Micromechanics

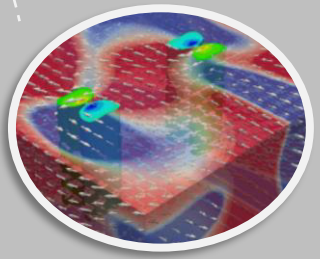
Numerical Meth.
- Finite element
- Finite difference



Energy Materials

- Battery materials
- Physical chemistry
- Chemomechanics

Rezaei et al. J. Mech. Phys. Solids. 2021
Luo et al. Nature Materials 2022
Projects: WV, DFG, CSC
MOOSE App under construction



Ferroic Materials

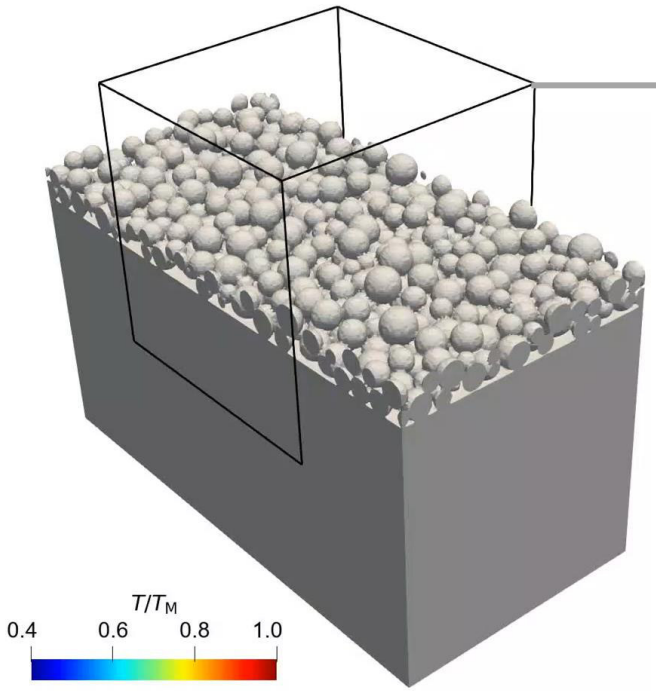
- Landau theory
- Micromagnetics
- Elasticity
- Electro- and magnetostatics

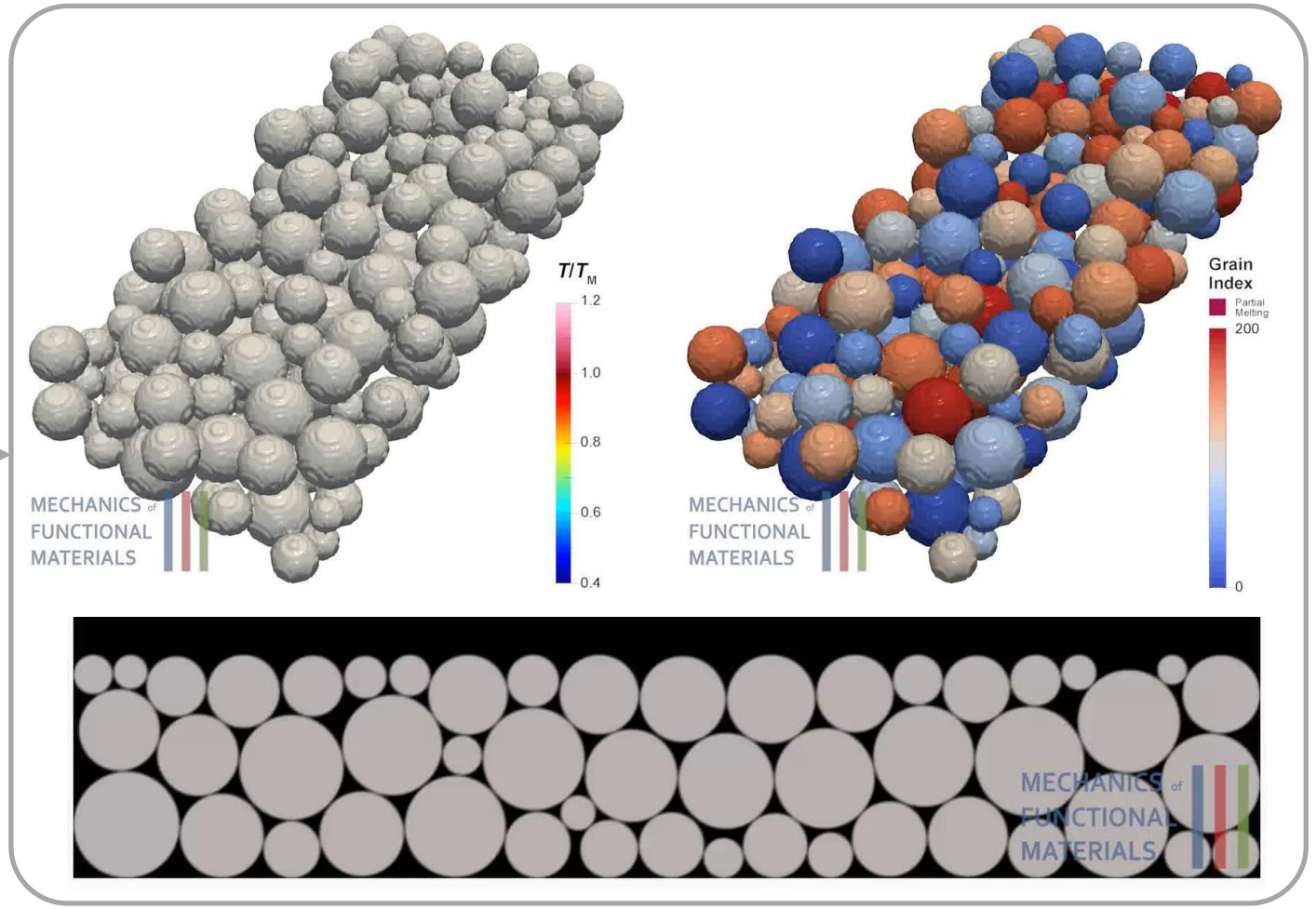
Höfling et al. Science 2021
Zhou et al. Int. J. Solids Struct. 2022
Höfling et al. Science 2021
Projects: TRR361, FLAME, RESPONSE
MOOSE App: **PMP**

MULTIPHYSICS MULTISCALE SIMULATOR 3D PRINTING

TECHNISCHE UNIVERSITÄT DARMSTADT

NIsoS
A MOOSE-BASED APPLICATION



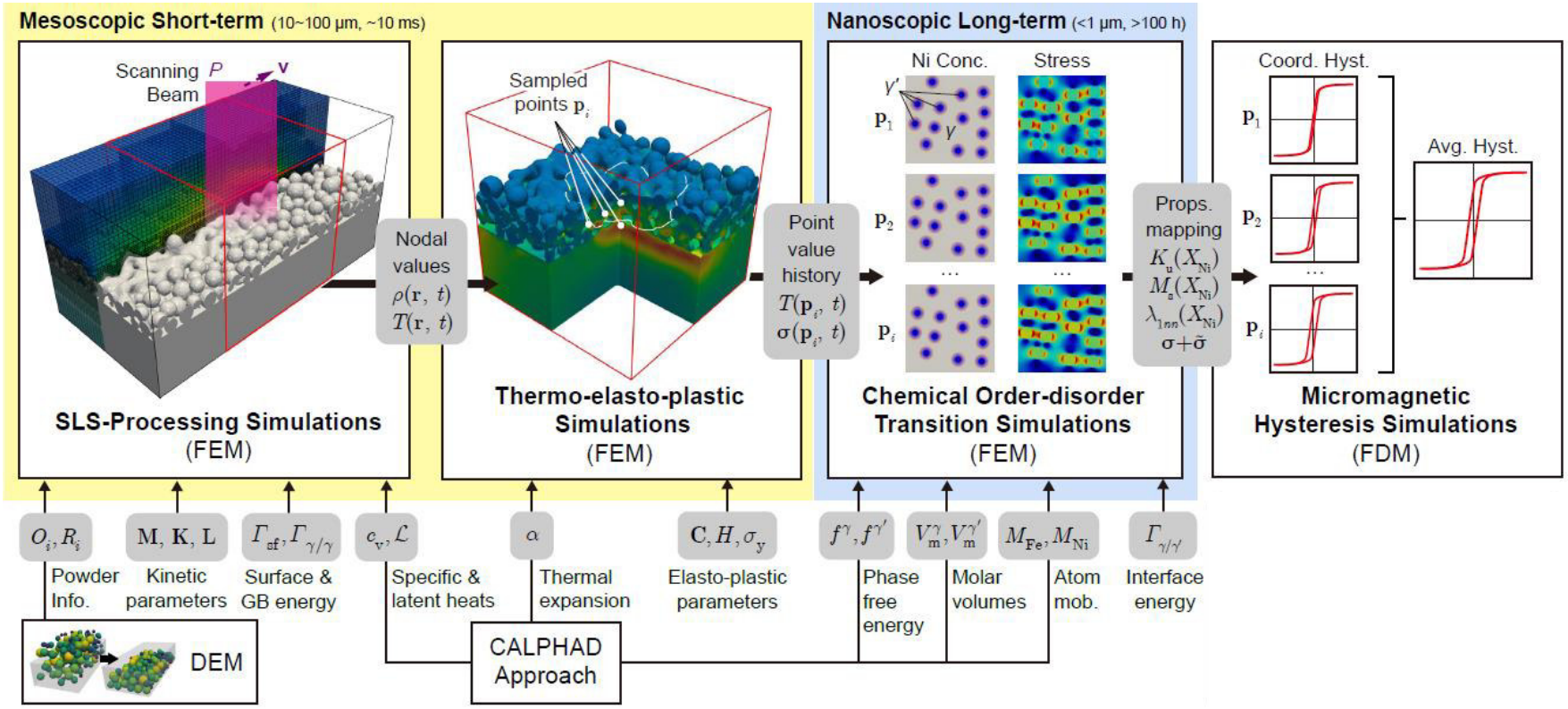


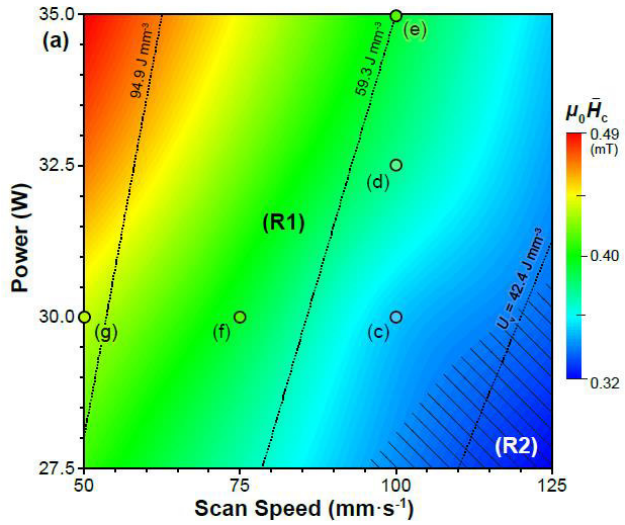
MECHANICS of FUNCTIONAL MATERIALS

MULTIPHYSICS MULTISCALE SIMULATOR PMP RELATION

TECHNISCHE UNIVERSITÄT DARMSTADT

NIsoS
A MOOSE-BASED APPLICATION

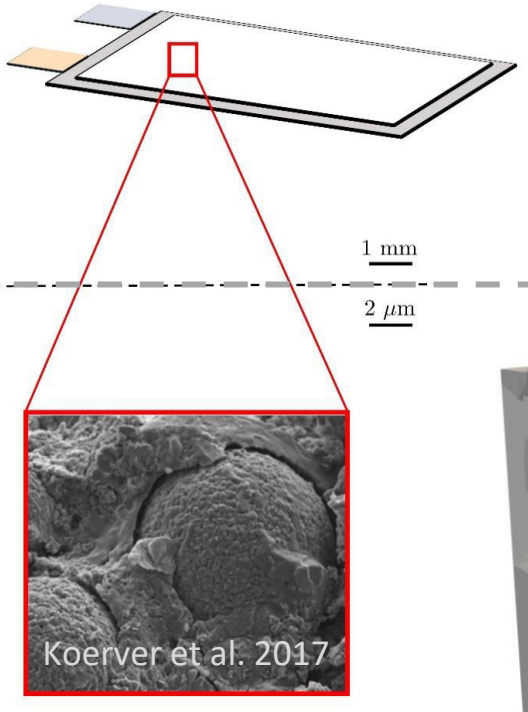


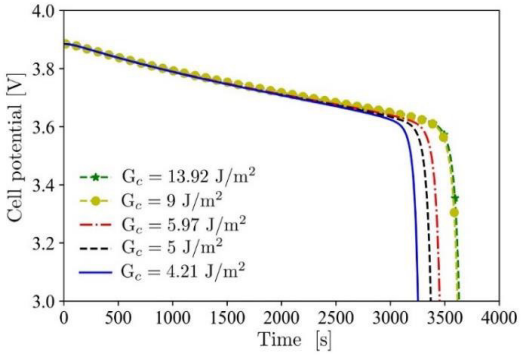


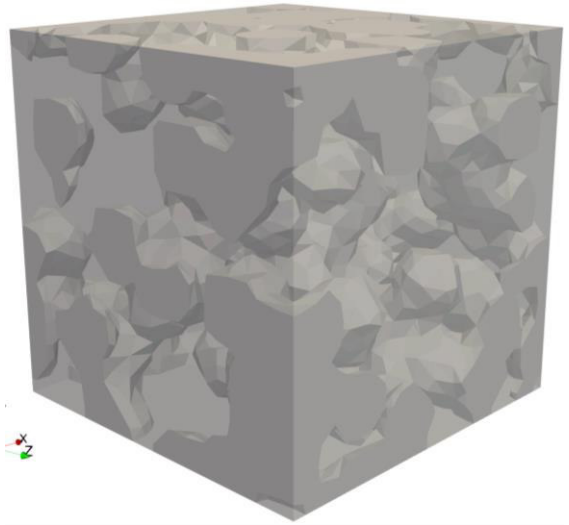
MECHANICS of FUNCTIONAL MATERIALS

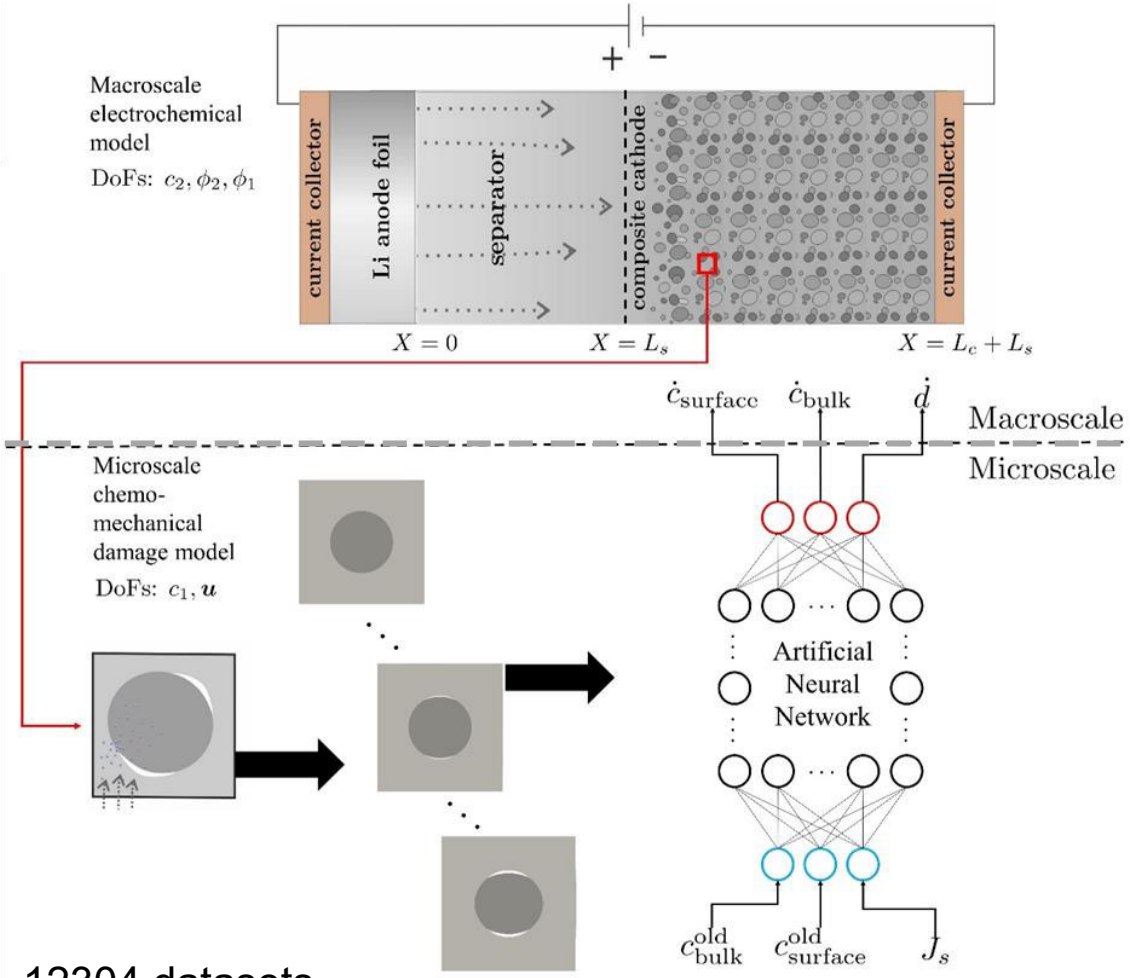
MULTIPHYSICS MULTISCALE SIMULATOR LITHIUM-ION BATTERY

TECHNISCHE UNIVERSITÄT DARMSTADT









12304 datasets

FE^2 (4 days) → FE+NN (20 min)

MECHANICS of FUNCTIONAL MATERIALS

MATERIAL-
WISSENSCHAFT

TECHNISCHE
UNIVERSITÄT
DARMSTADT

TU DARMSTADT & MERCK KGAA – ORGANISCHE ELEKTRONIK

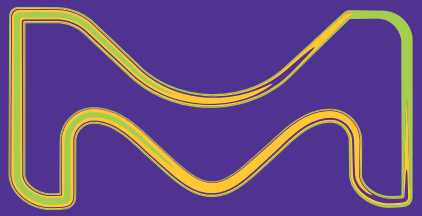
Prof. Dr. Peer Kirsch

Merck Electronics & organic electronic@TUDa

Industrietag Materialwissenschaft

Prof. Dr. Peer Kirsch, Merck Electronics KGaA & TU Darmstadt
17 Nov 2023





Merck



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Merck Electronics

Merck KGaA, Darmstadt, Germany holds the rights to the name and trademark "MERCK" internationally, except for the United States and Canada.



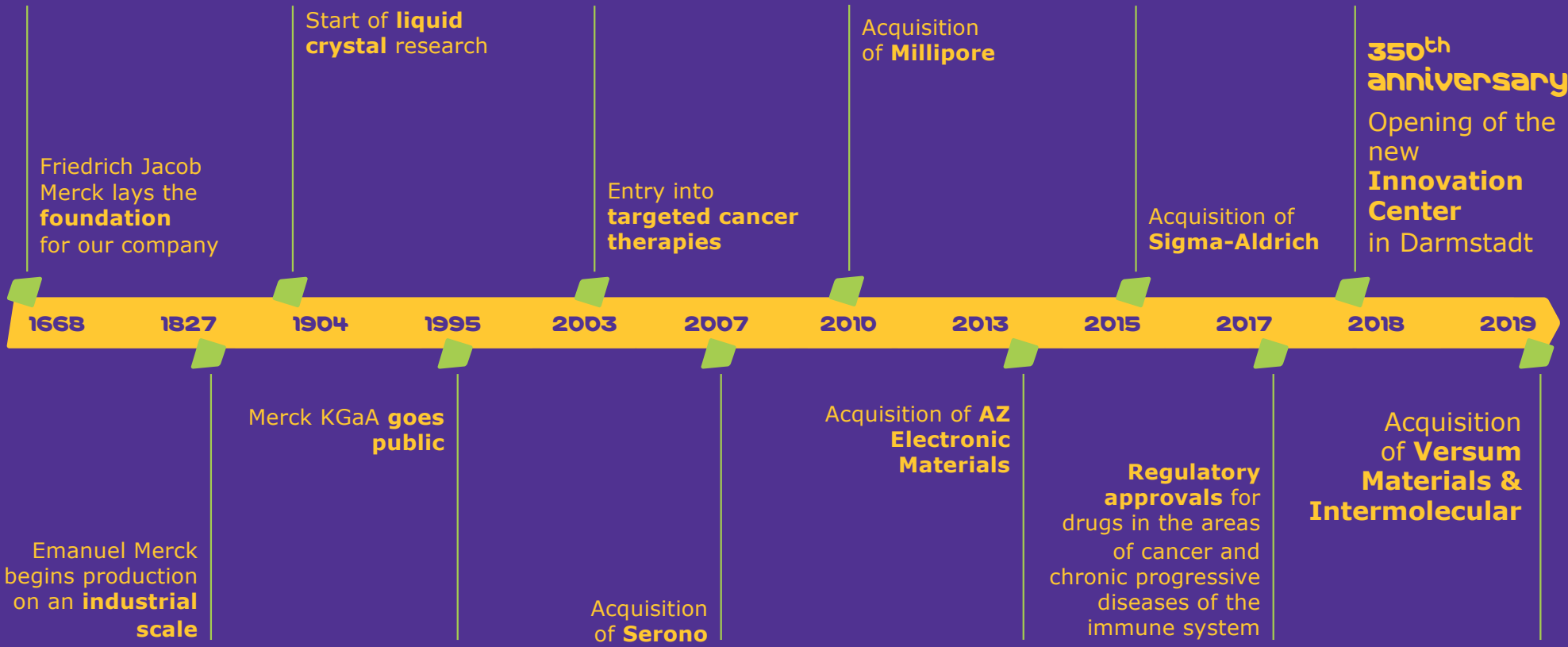
we are unique

Every day, our nearly 60,300 employees work in 66 countries to make a positive difference to millions of people's lives by creating more joyful and sustainable ways to live.

EMD Serono MilliporeSigma EMD Electronics

In the U.S. and Canada we operate as EMD Serono in the biopharmaceutical business, MilliporeSigma in the life science business, and EMD Electronics in the high-tech materials business.

Over 350 Years of curiosity



We have 3 high-tech business sectors competing in attractive markets

Healthcare



Leading in specialty pharma markets

- Biologics and small-molecule **prescription medicines** against cancer, multiple sclerosis, infertility
- **Research** focus: Oncology, Immunology & Immuno-Oncology

Life Science



Leading in life sciences

- Tools and services for **biotech research & production**
- **Tools and laboratory supply** for academic research and industrial testing

Electronics

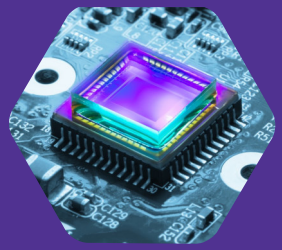


Leading in high-tech solutions

- High-tech solutions and materials for **electronics**
- Broad portfolio of **decorative and functional solutions**

Our Businesses

Semiconductor Solutions



Semiconductor Materials

are at the heart of Electronics and enable the transformation of communications, mobility and healthcare. We unlock the potential for smaller, faster, and more powerful devices.



Delivery Systems & Services

safely guards the molecule of semiconductor and display materials. We provide high-quality delivery and storage of specialty chemicals and gases.

Display Solutions



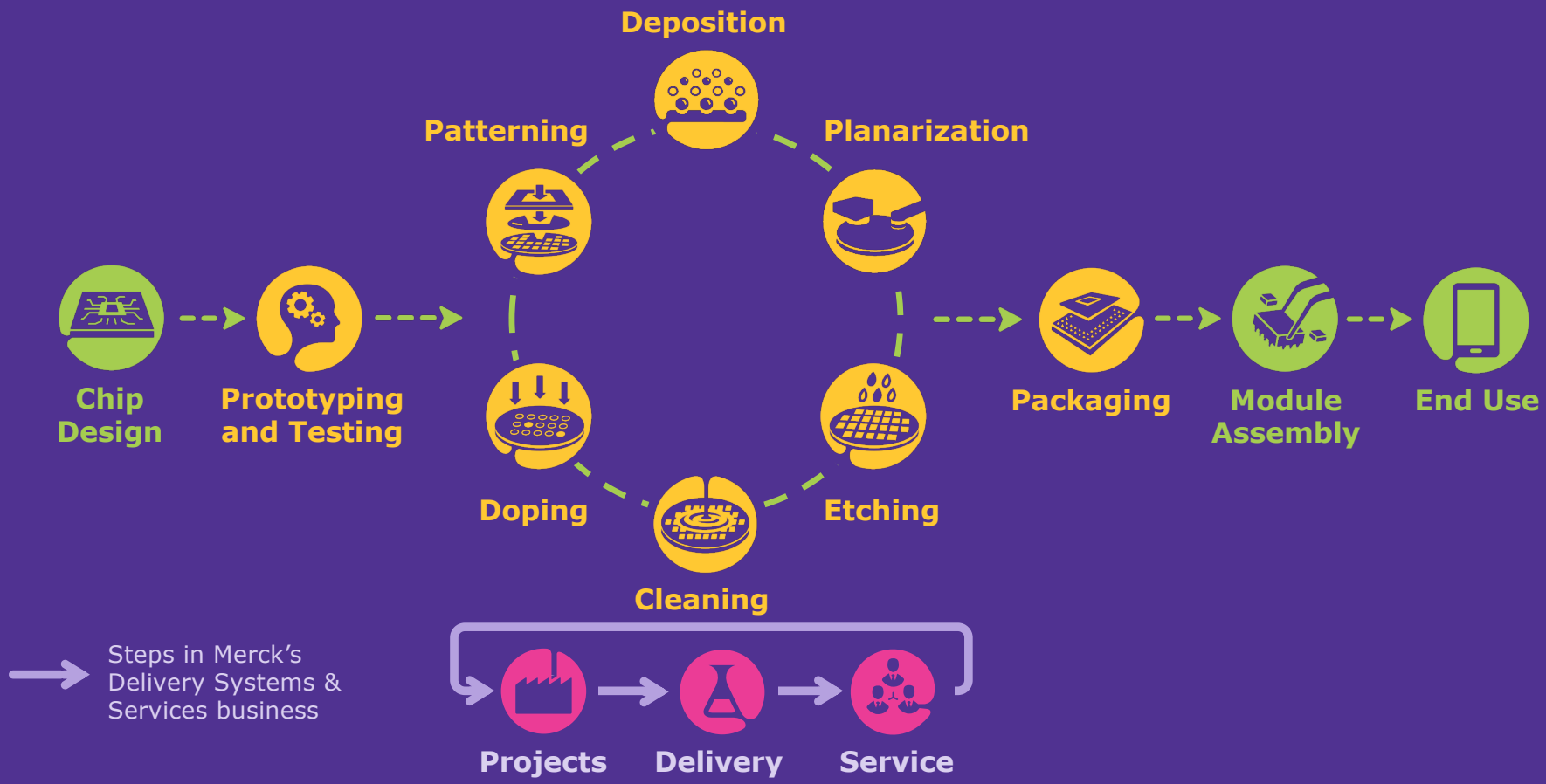
offers next generation material, equipment systems and services that revolutionize Electronics. We help to connect the intelligence inside devices with human experience.

Surface Solutions



helps redefine the use of color in modern living. Our broad portfolio of pigments and active ingredients continue to drive value in the Automotive, Cosmetic and Industrial industries.

As a trusted partner, we are delivering **Integrated Materials Solutions** to speed innovation





2002



2010



2000



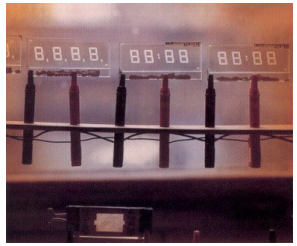
1995



1990



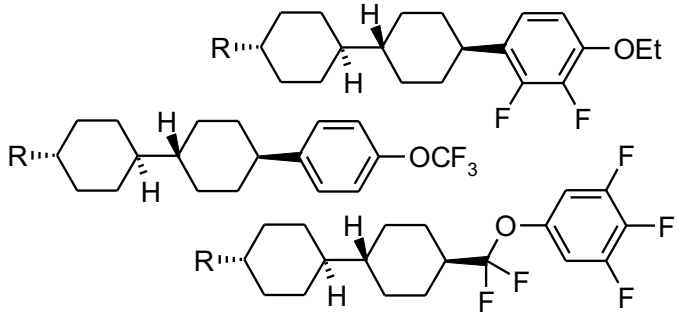
1973



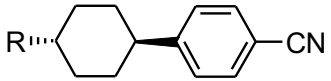
1968



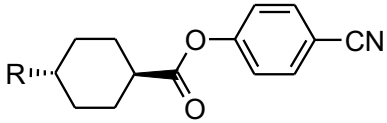
1966



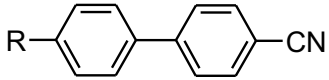
"Super Fluorinated Materials" (SFM), **1985+**



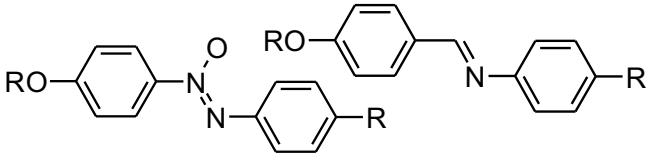
R. Eidenschink *et al.*, **1976**

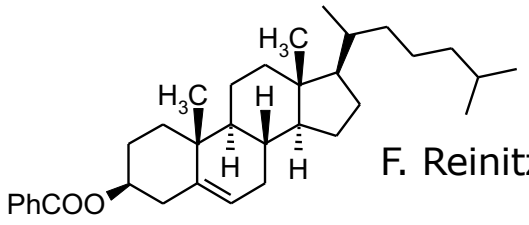


D. Demus *et al.*, **1975**



G. W. Gray *et al.*, **1972**





F. Reinitzer, **1888**

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organische Elektronik @ TUDa

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The Limits of Computation
Energy Consumption

ENERGY SCALE

Global electricity demand

20,000 TWh

Electricity use by ICT

2,000 TWh

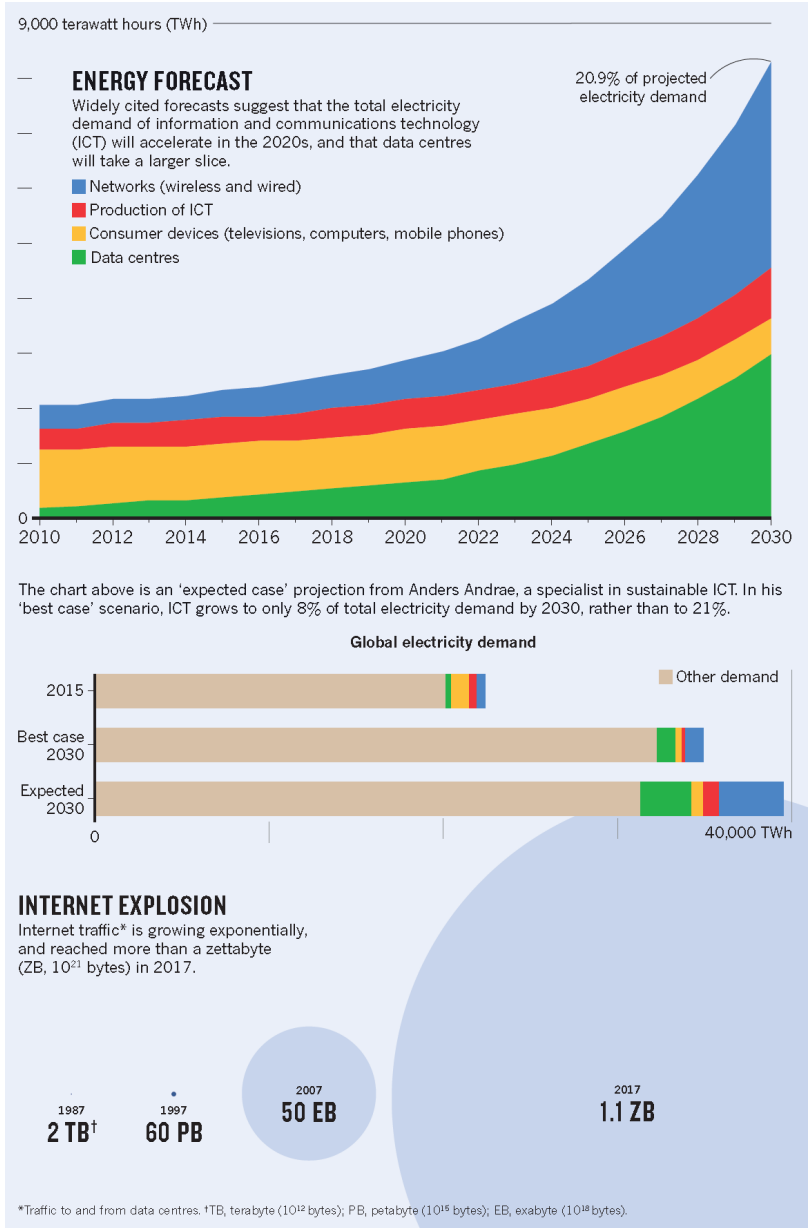
Data-centre electricity demand

200 TWh

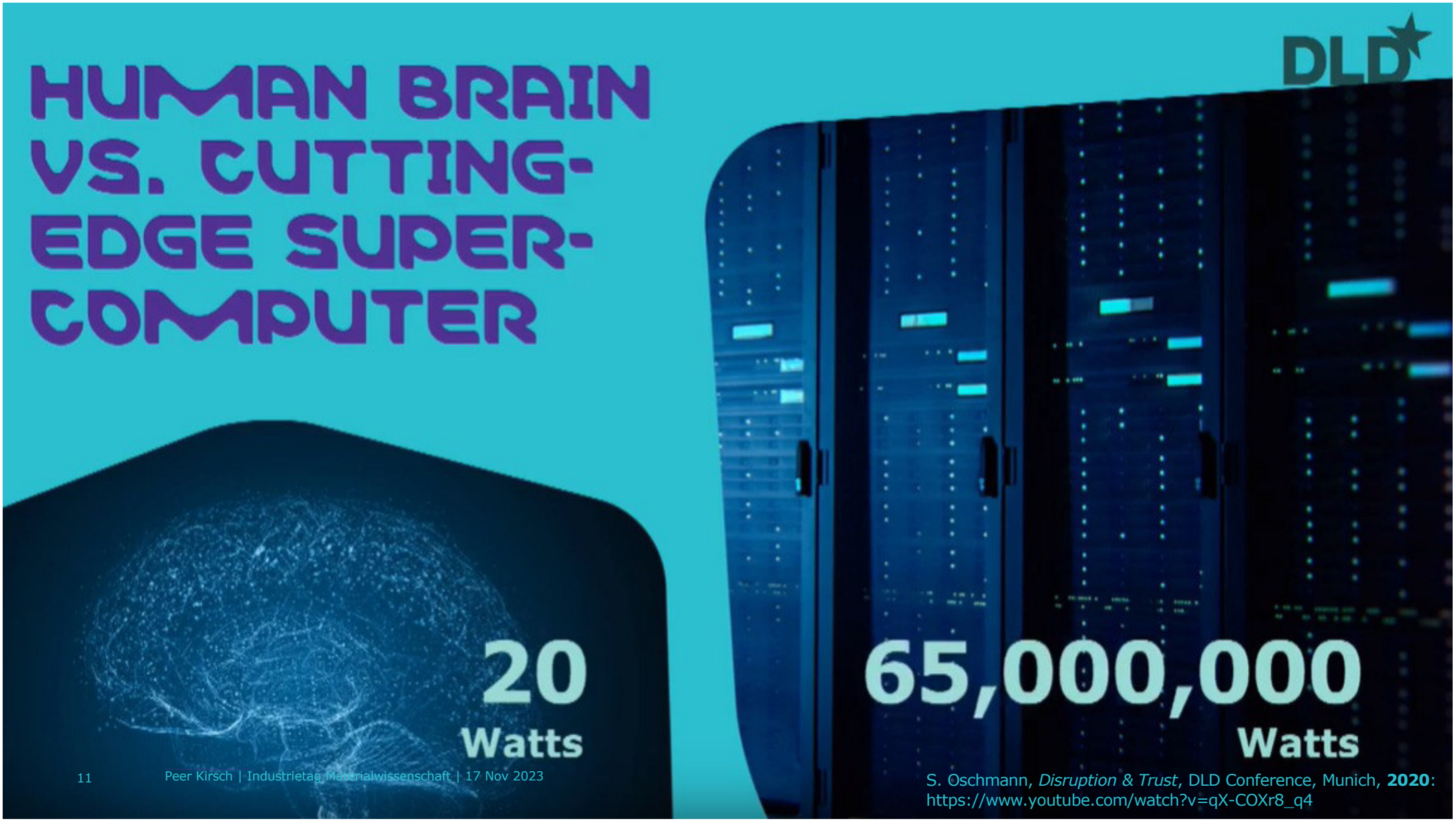
Bitcoin use by mid-2018

20 TWh

Figures are approximate.

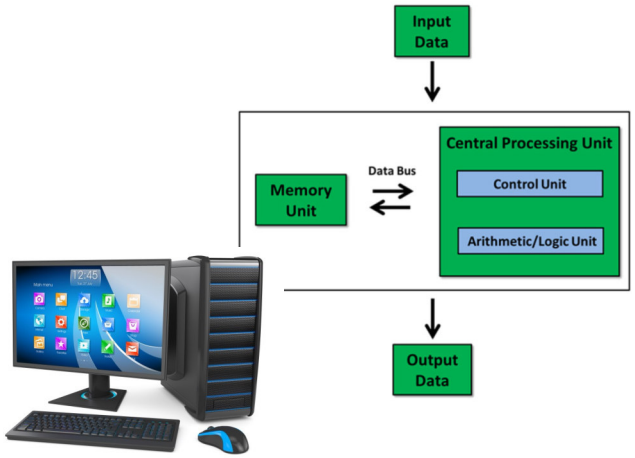


N. Jones, *Nature* **2018**, *561*, 163-166

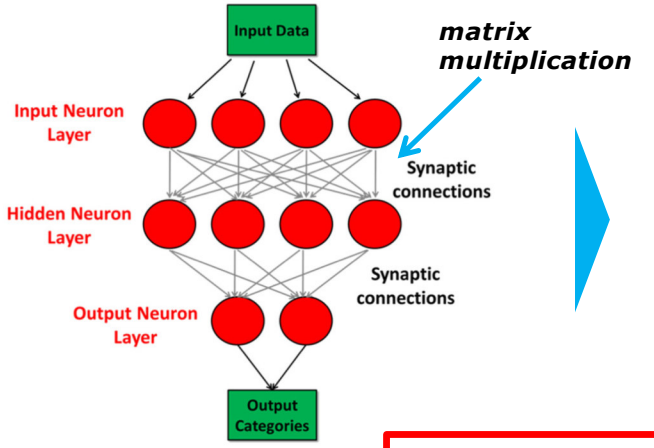


S. Oschmann, *Disruption & Trust*, DLD Conference, Munich, **2020**: https://www.youtube.com/watch?v=qX-COXr8_q4

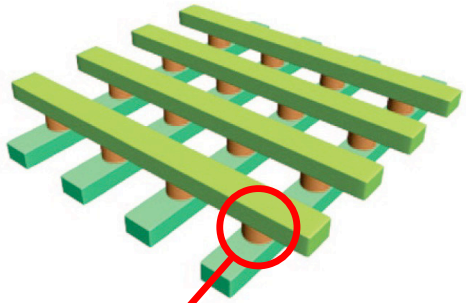
von Neumann Architecture

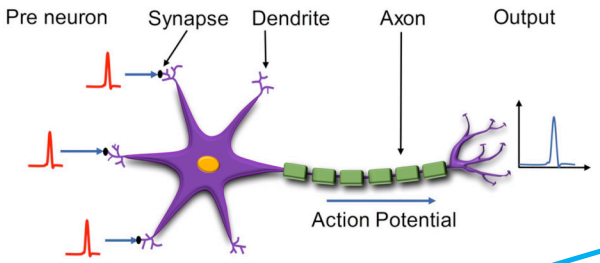


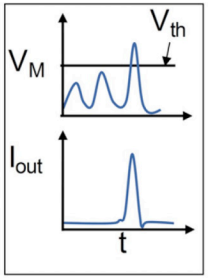
Neuromorphic Architecture



Crossbar Array

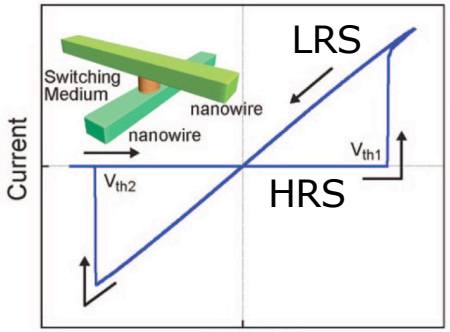






integration, threshold detection

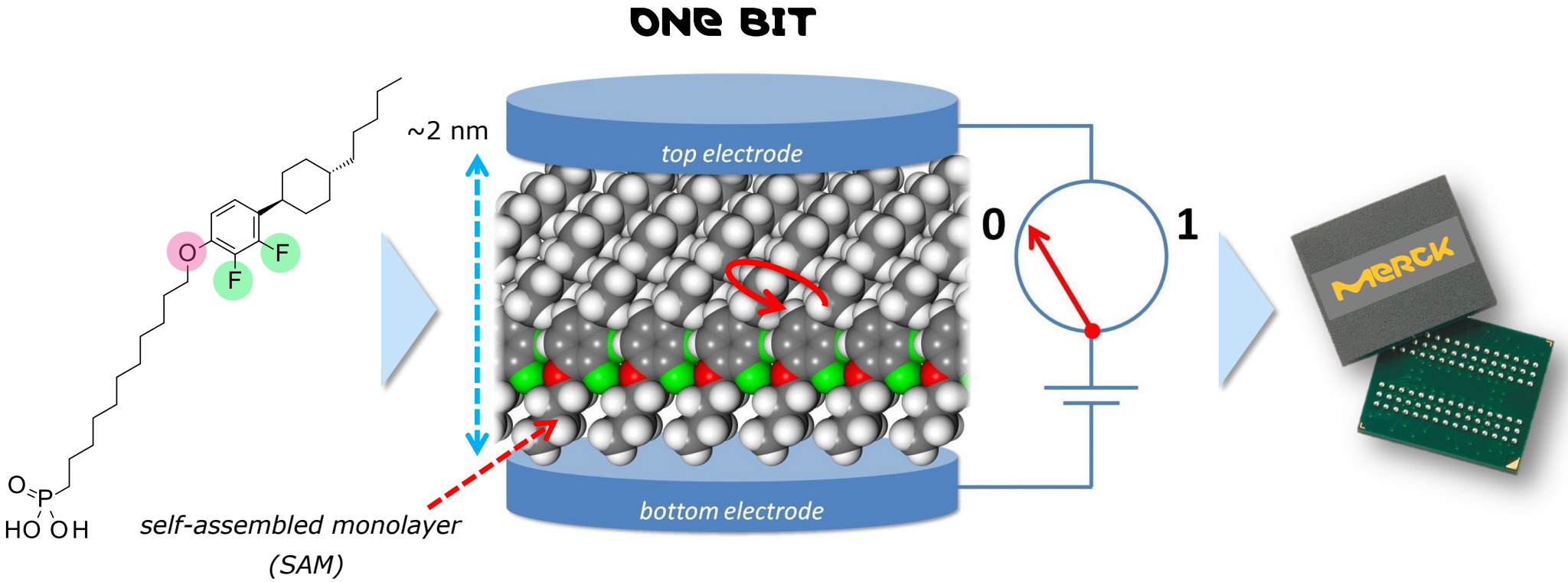
Memristor



Novel materials required

J. del Valle, J. G. Ramirez, M. J. Rozenberg, I. K. Schuller, *J. Appl. Phys.* **2018**, *124*, 211101 (doi: 10.1063/1.5047800); H. Kalita, A. Krishnaprasad, N. Choudhary, S. Das, D. Dev, Y. Ding, L. Tetard, H.-S. Chung, Y. Jung, T. Roy, *Sci. Rep.* **2019**, *9:53* (doi: 10.1038/s41598-018-35828-z); S. H. Jo, K.-H. Kim, W. Lu, *Nano Lett.* **2009**, *9*, 870-874 (doi: 10.1021/nl8037689).

Integration of Liquid Crystal Technology into Semiconductor Devices



J. Dlugosch, H. Seim, A. Bora, T. Kamiyama, I. Lieberman, F. May, F. Müller-Plathe, A. Nefedov, S. Prasad, S. Resch, K. Saller, C. Seim, M. Speckbacher, F. Voges, M. Tornow, P. Kirsch, *ACS Appl. Mater. Interfaces* **2022**, *14*, 31044-31053 (doi: 10.1021/acsami.2c05264)

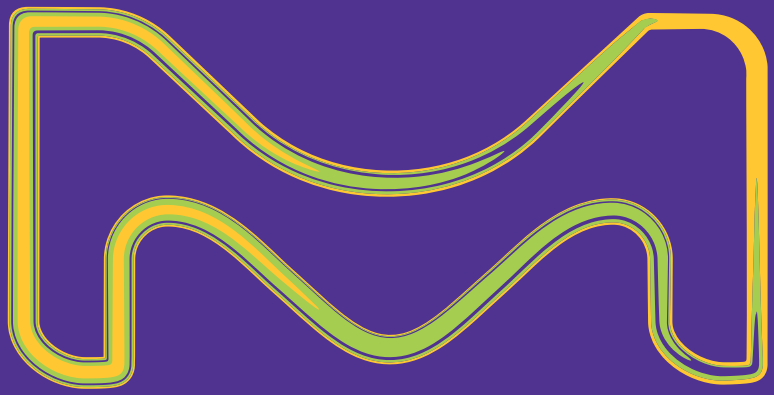


P. Kirsch,
Labor & More **2013** (5), 44-49

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64293 Darmstadt
Germany

peer.kirsch@merckgroup.com



MATERIAL-
WISSENSCHAFT

TECHNISCHE
UNIVERSITÄT
DARMSTADT

OFFENER AUSTAUSCH IN L2|01

Das Hauptgebäude des Instituts für Materialwissenschaft befindet sich nebenan.