MSE Day

November 5th, 2024

Information-Based Materials Systems Engineering Along All Process Chains

P3T1 Functionality by Information Guided Design

Jasmin Aghassi-Hagmann

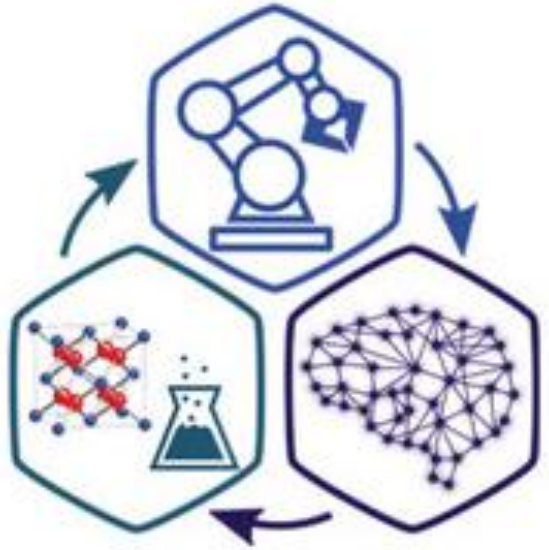
Topic Spokesperson

HELMHOLTZ Information

Functionality by information guided design

Mission: Design, prediction and control of material functions from molecular to device level

- **Digital twins (closed loop theory/experiment)**
- **AI-guided prediction and materials design**
- **High throughput synthesis and characterization**

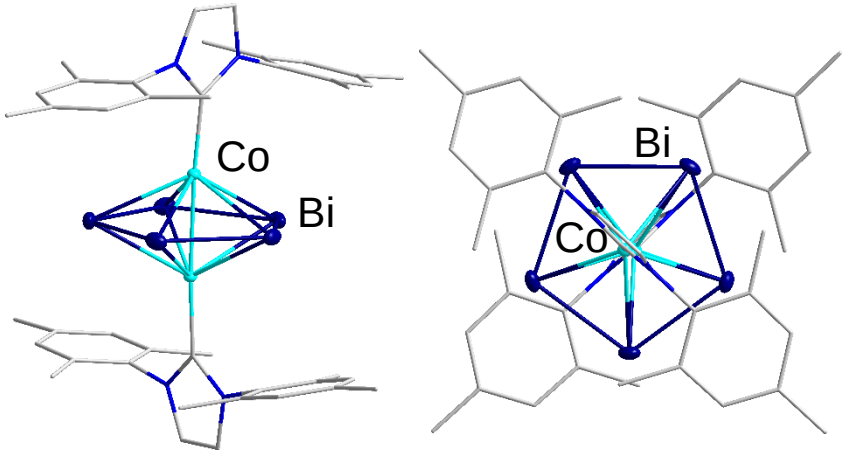


- **Exploration of novel materials and devices for information technology**

Research Highlight (I): Digital Twins

Design and synthesis of aromatic metal clusters

- Demonstration of first of its kind synthetic metal Bi_5 complexes
- Closed loop theory (DFT) and experiment

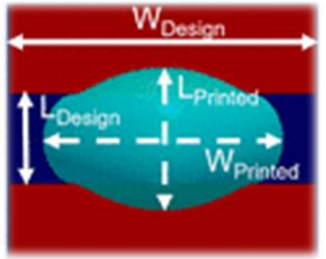


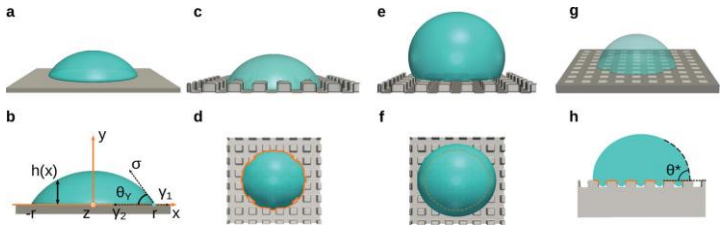
$[(IMesCo)_2Bi_5]$ *Nat. Chem.* **2024**, *accepted*

Dehnen, Weigend, Wernsdorfer (P3T1/P1)

Wetting phenomena on patterned substrates

- Prediction of shape, wetting angle and physical design

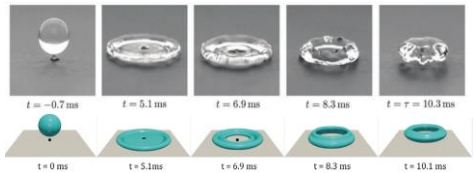




Langmuir. **2024**, *15,* 347–356 *Adv. Mat.* **2023**, *35, 2210745*

Phys. Rev. Lett. **2024**, 132, 126202 *Phys. Rev. Lett.* **2024**, accepted

Droplet dynamics on solid substrates



JOINT LAB VIRTUAL MATERIALS DESIGN

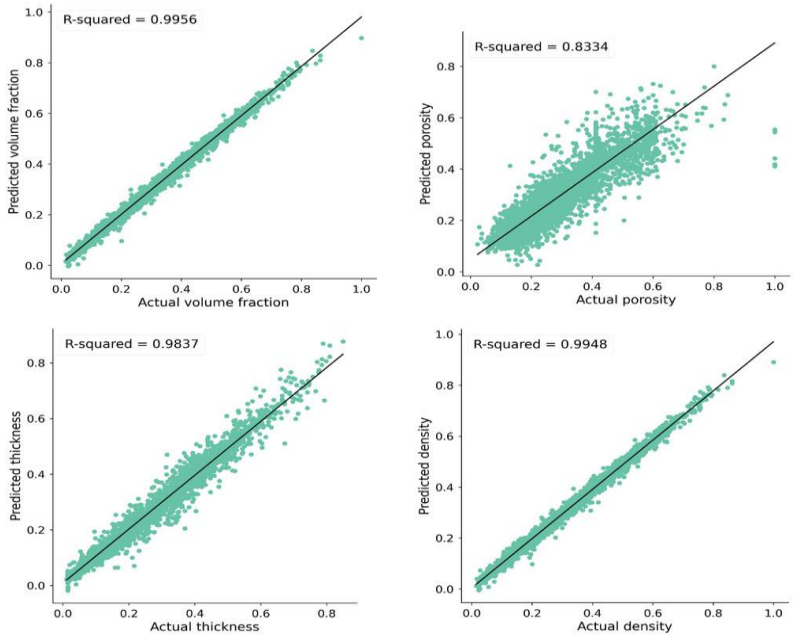
Adv. Mater. 2021, Soft Matter 2024, J. Chem. Phys. 2023

Nestler, Wang, Levkin, Aghassi (P3T1/P3T3)

Research Highlight (II): Virtual Materials Design

Virtual material design for solid electrolyte interphases

- Data-driven strategy to improve the understanding of SEI formation
- Prediction of real, physical properties from neural network based Variational AutoEncoders



Adv. Energy Mater. **2023**, 13 (40), 2301985

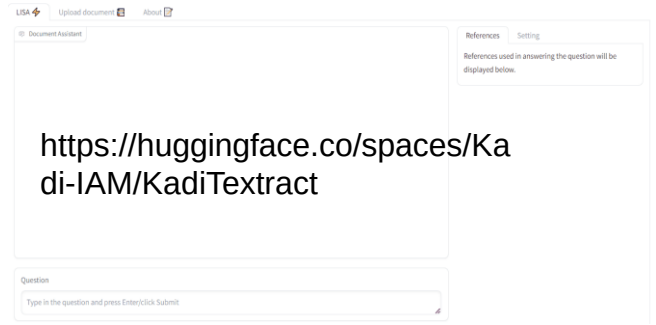
Nestler, Selzer, Stein, Wenzel

POLiS Post Lithium Storage Cluster of Excellence

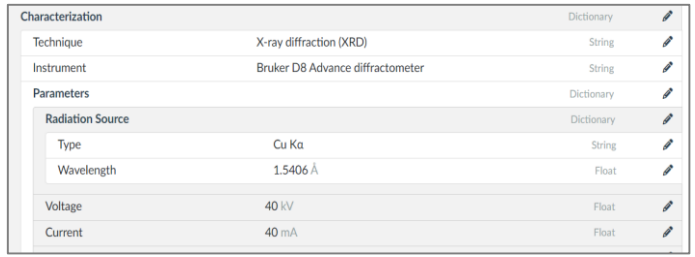
KadiAI incorporates LLM Research Assistant

- Chat with scientific documents

https://huggingface.co/spaces/Kadi-IAM/KadiTextract



- Automate knowledge extraction, visualization, and analysis



Koeppe, Schneider, Selzer

Research Data Infrastructure

Kadi4Mat Karlsruhe Data Infrastructure for Materials Science

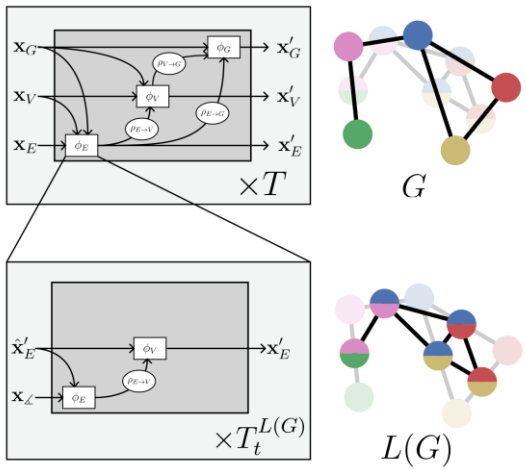
JOINT LAB VIRTUAL MATERIALS DESIGN

HELMHOLTZ Information

Research Highlight (III): AI-guided materials properties predictions

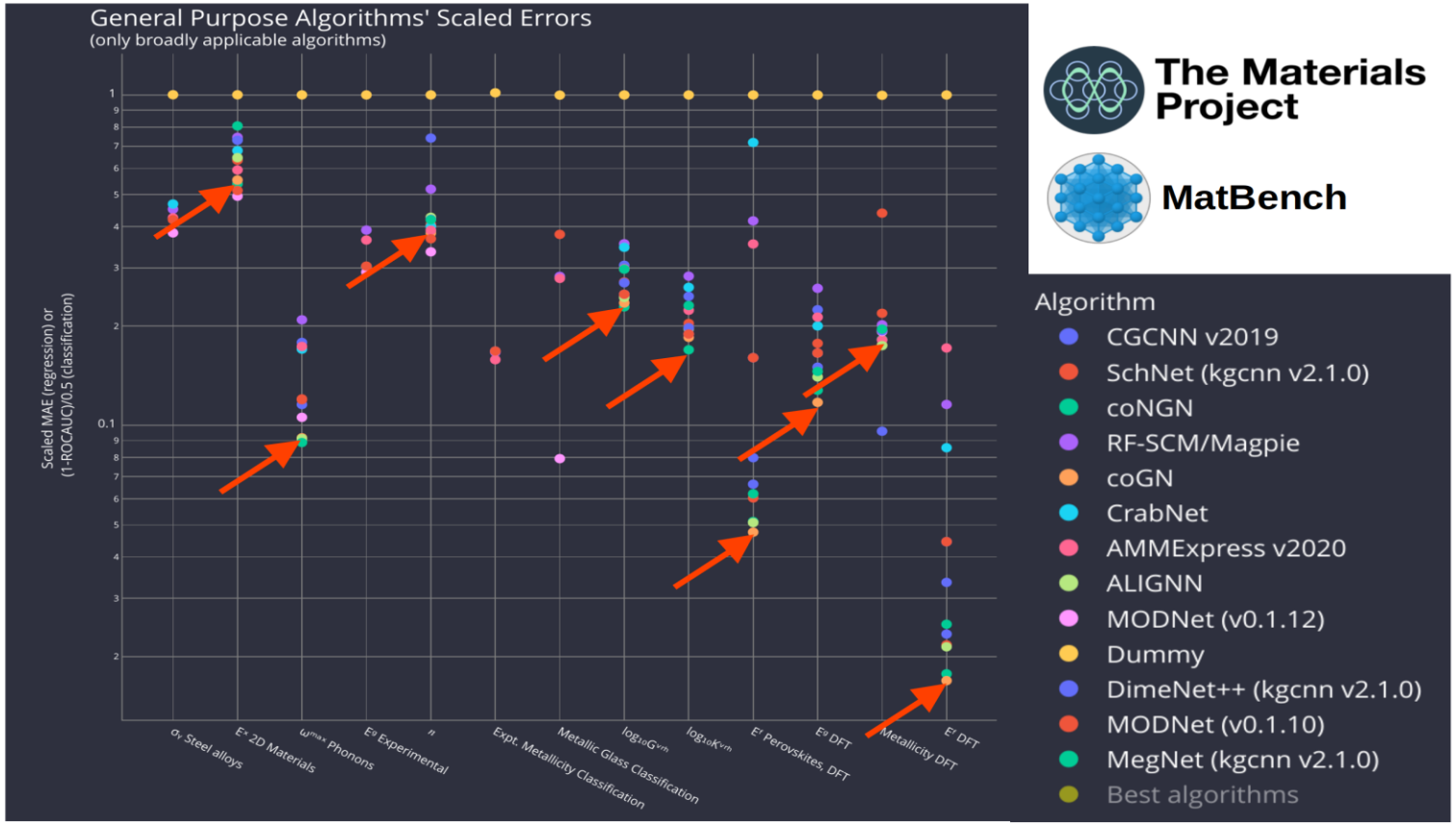
Graph neural networks

- Properties prediction of stability, defects
- Surface reaction kinetics
- Understanding of particle interactions in disordered, amorphous, polycrystalline materials, in solid and liquid systems



Ruff *et al.*, coNGN, NeurIPS AI4Mat 2023, https://arxiv.org/abs/2302.14102

KIT model wins benchmarks:



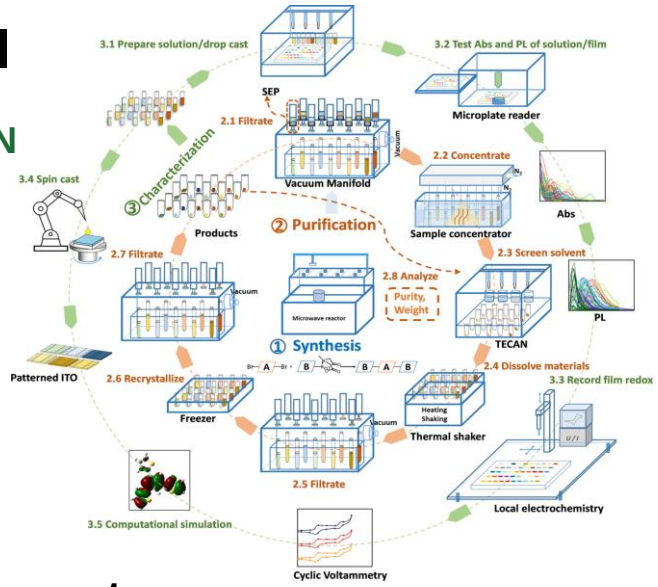
Friederich group

Research Highlight (III): AI-guided materials properties predictions

Solar cell material

Collaboration with HI-ERN

Wu *et al.*, JACS 2023
Wu *et al.*, u. review 2024

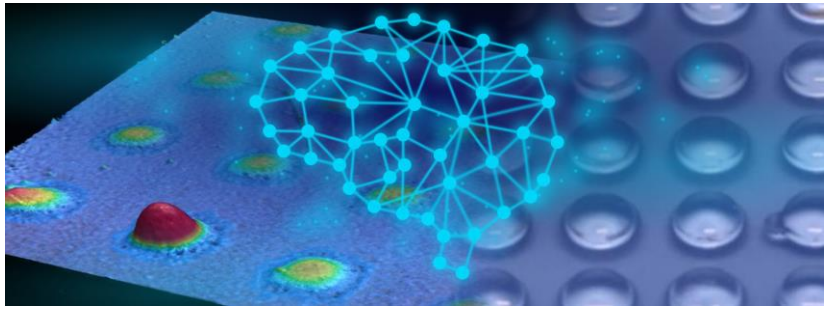


Friedrich-Alexander-Universität Erlangen-Nürnberg

Responsive polymers

Collaboration with P3T3, Levkin group

Seifermann *et al.*, Small Methods 2023.



Catalyst development

Collaboration: HI-ERN

Jenewein *et al.*, J. Mat. Chem. A 2023

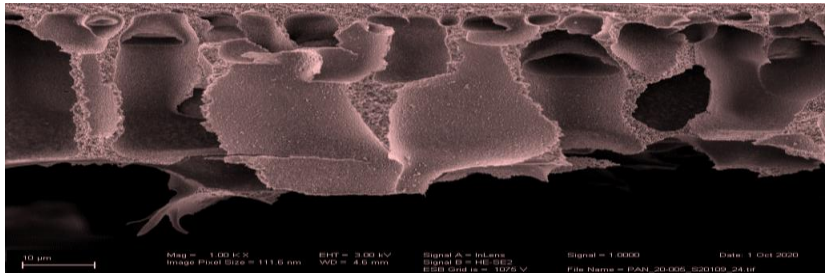
HI ERN Helmholtz Institute Erlangen-Nürnberg part of Forschungszentrum Jülich

Navigating the unknown with AI: multiobjective design for catalyst activity and catalyst stability

Filtration membrane design

Collaboration: Hereon

Glass *et al.*, ACS Applied Materials & Interfaces 2024

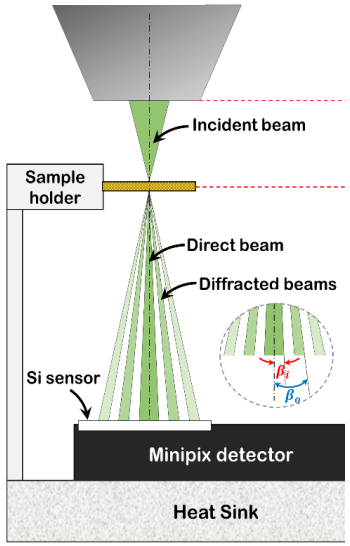


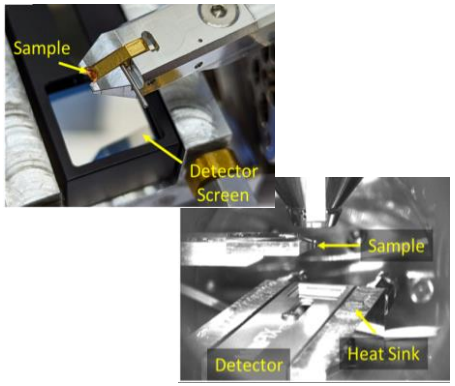
Research Highlight (IV): Highthroughput Characterization

Kirchlechner group and Subin Lee

4D STEM-SEM:

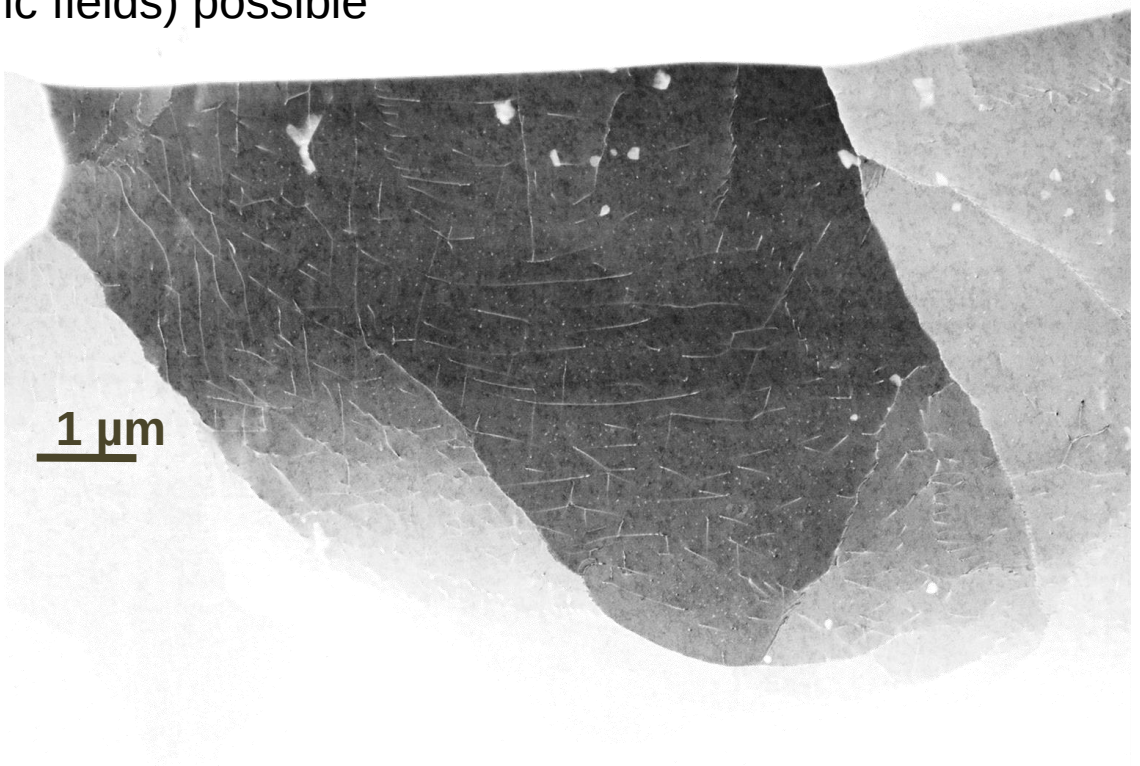
- 4D-Scanning Transmission Electron Microscopy in the SEM, 2D real space scanning and 2D reciprocal space imaging
- Rich data (phase, orientation, strain resolved via postprocessing)
- Operated in event mode for significant data reduction and acceleration
- In situ triggers (strain, temperature, electric fields) possible





Electron Channeling Contrast Imaging: cECCI

- High throughput imaging of lattice defects
- Imaging dislocations in the SEM
- Burgers vector analysis
- Fundamental understanding of material mechanics
- Mechanism based alloy design
- Unprecedented large areas and sound statistics



Research Highlight (V): High Entropy Materials for Information Technology and Energy Devices

Change in Gibbs free energy by change in enthalpy and configurational entropy

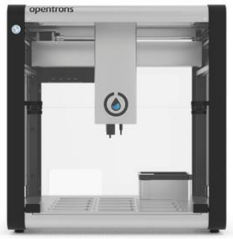
$$\Delta G = \Delta H - T\Delta S_{config}$$

$S_{config} > 1.5\ R \rightarrow$ High Entropy

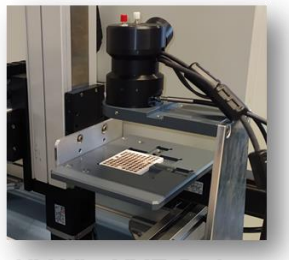
Enthalpy of mixing (ΔH_{mix})

Configurational entropy (ΔS_{config})

High throughput platform (Auto.Map):

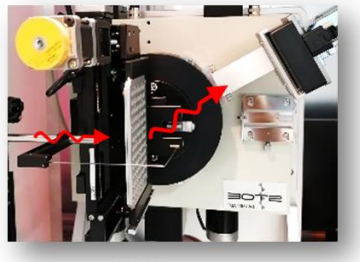


Synthesis, mixing, drop casting

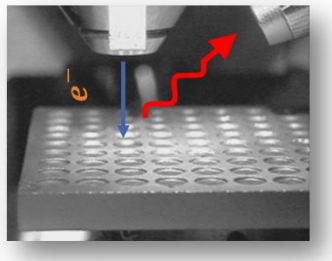


UV-Vis XYZ-Robot

Electrochemical characterization XYZ-robot equipped with SDC



XRD



SEM-EDX

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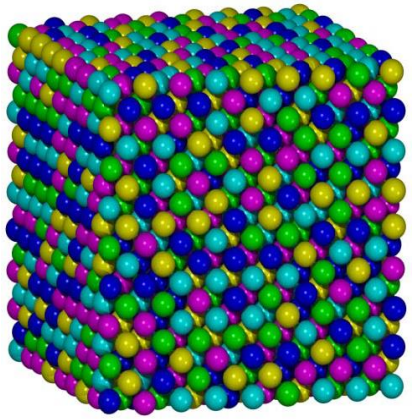
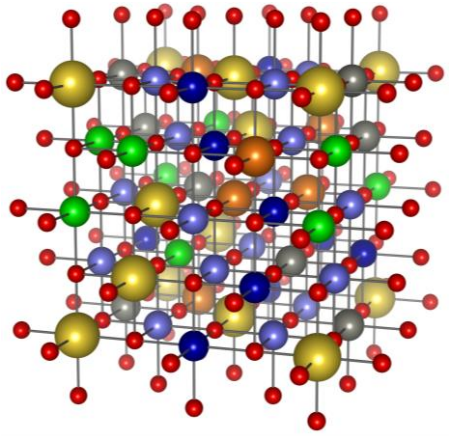
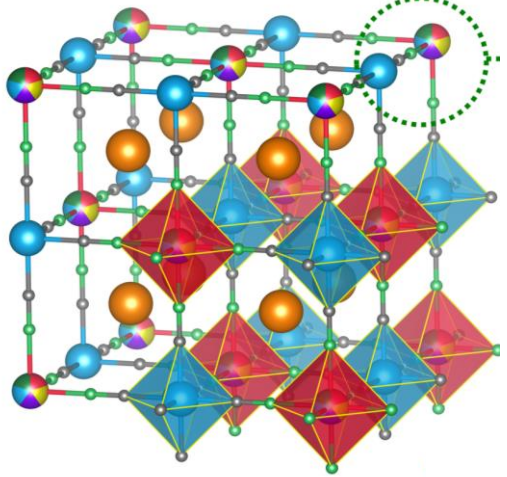


HEA



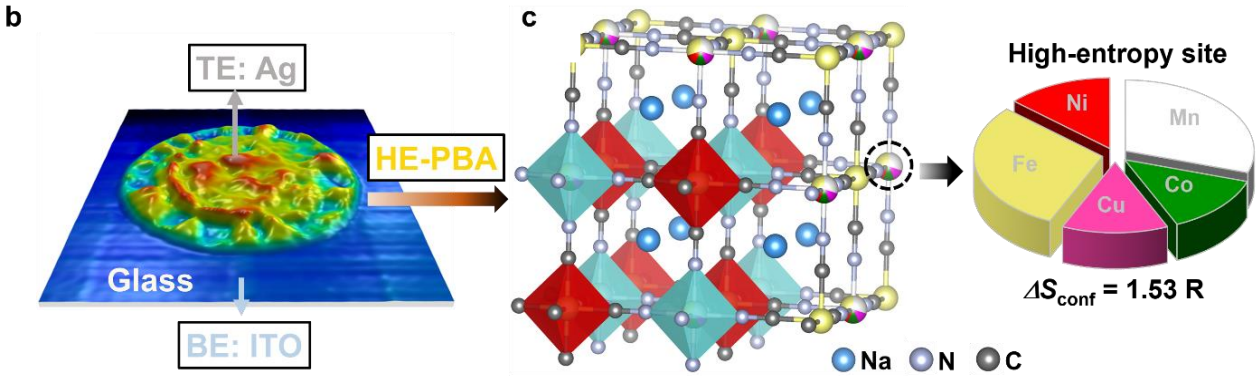
HEC



HE-MOF

Nature Reviews Materials, 9, 266–281 (2024)

Printable HE-PBA Memristor



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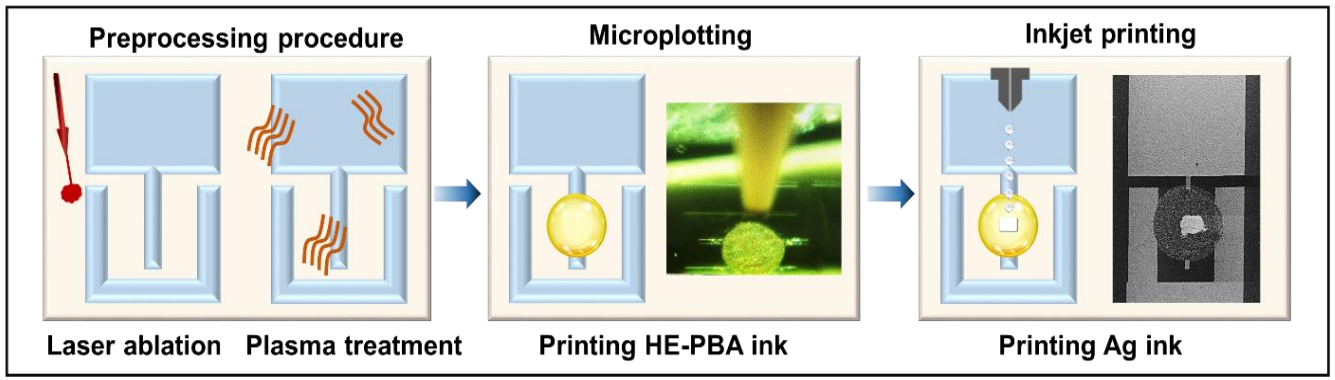
Materials	Measured atomic ratio
HE-PBA	$Na_{1.38}Mn_{0.3}Fe_{0.3}Co_{0.133}Ni_{0.133}Cu_{0.133}[Fe(CN)_6]_{0.84}\square_{0.16}\cdot 0.92H_2O$

Fabrication process of an Ag/HE-PBA/ITO stack

- Microplotting of HE-PBA
- Inkjet printing of silver electrode
- Laser structured ITO electrode

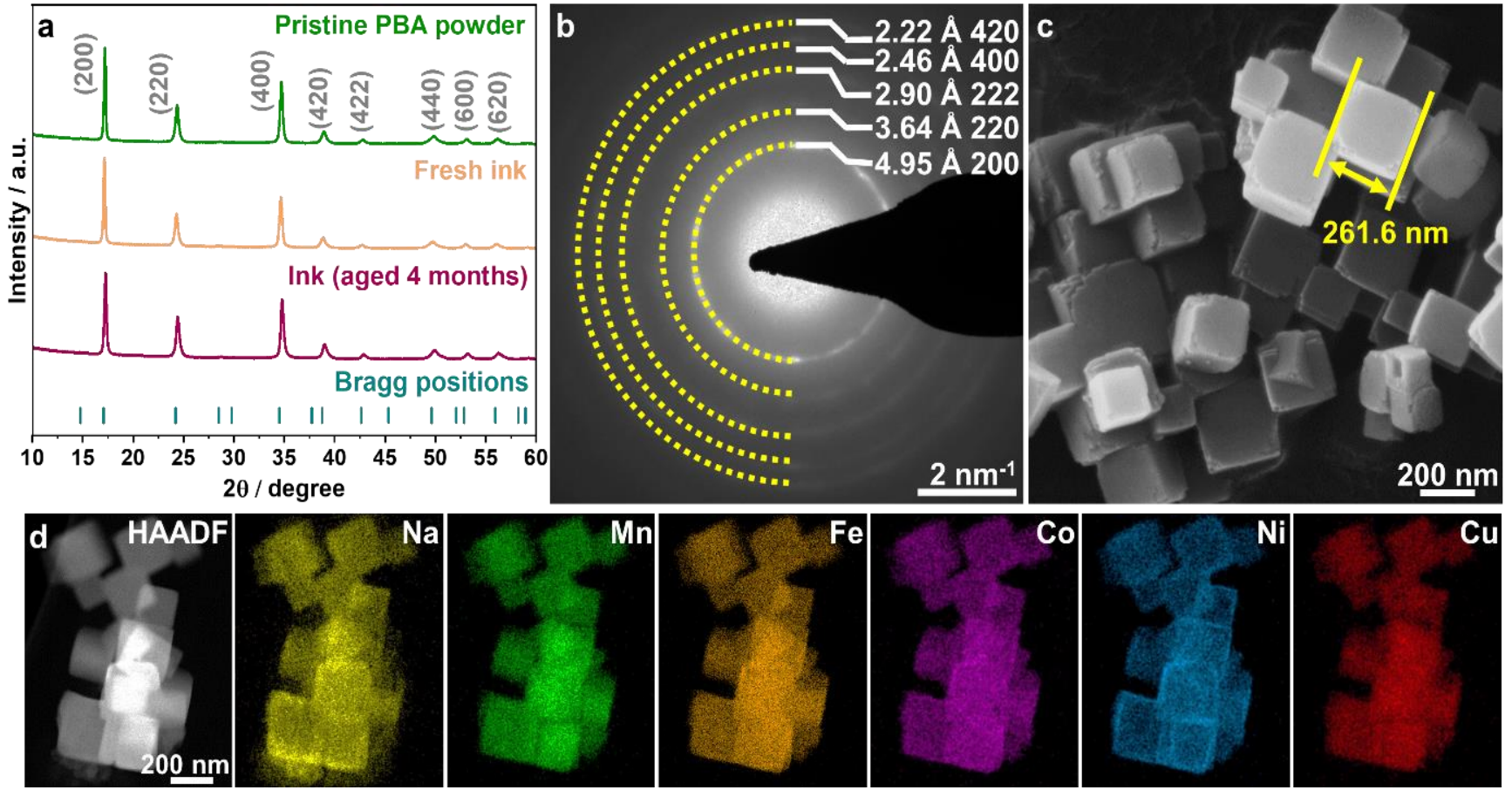


Adv. Mat. 2024, accepted

Structural and Morphological Characterization

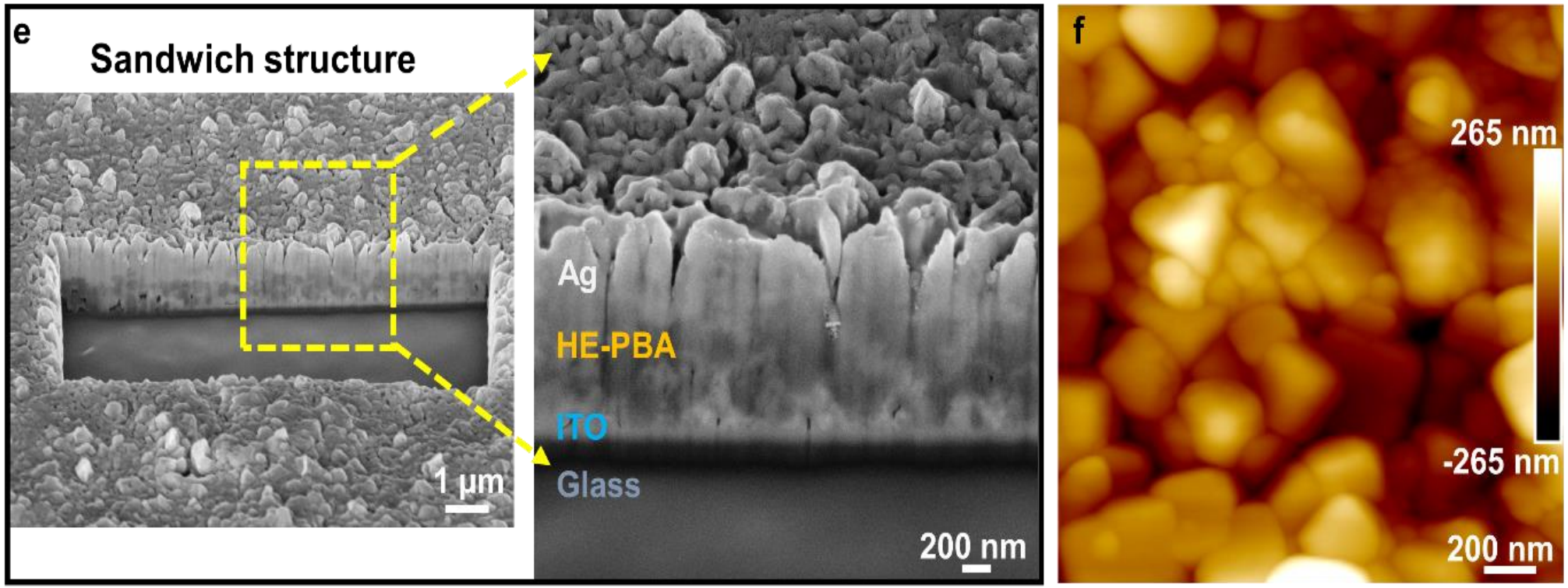
TEM studies reveal

- fcc lattice
- no difference between pristine and dispersed HE-PBA
- cubic HE-PBA nanoparticles
- Good aging properties



Adv. Mat. 2024, accepted

Device SEM cross-section and AFM surface studies

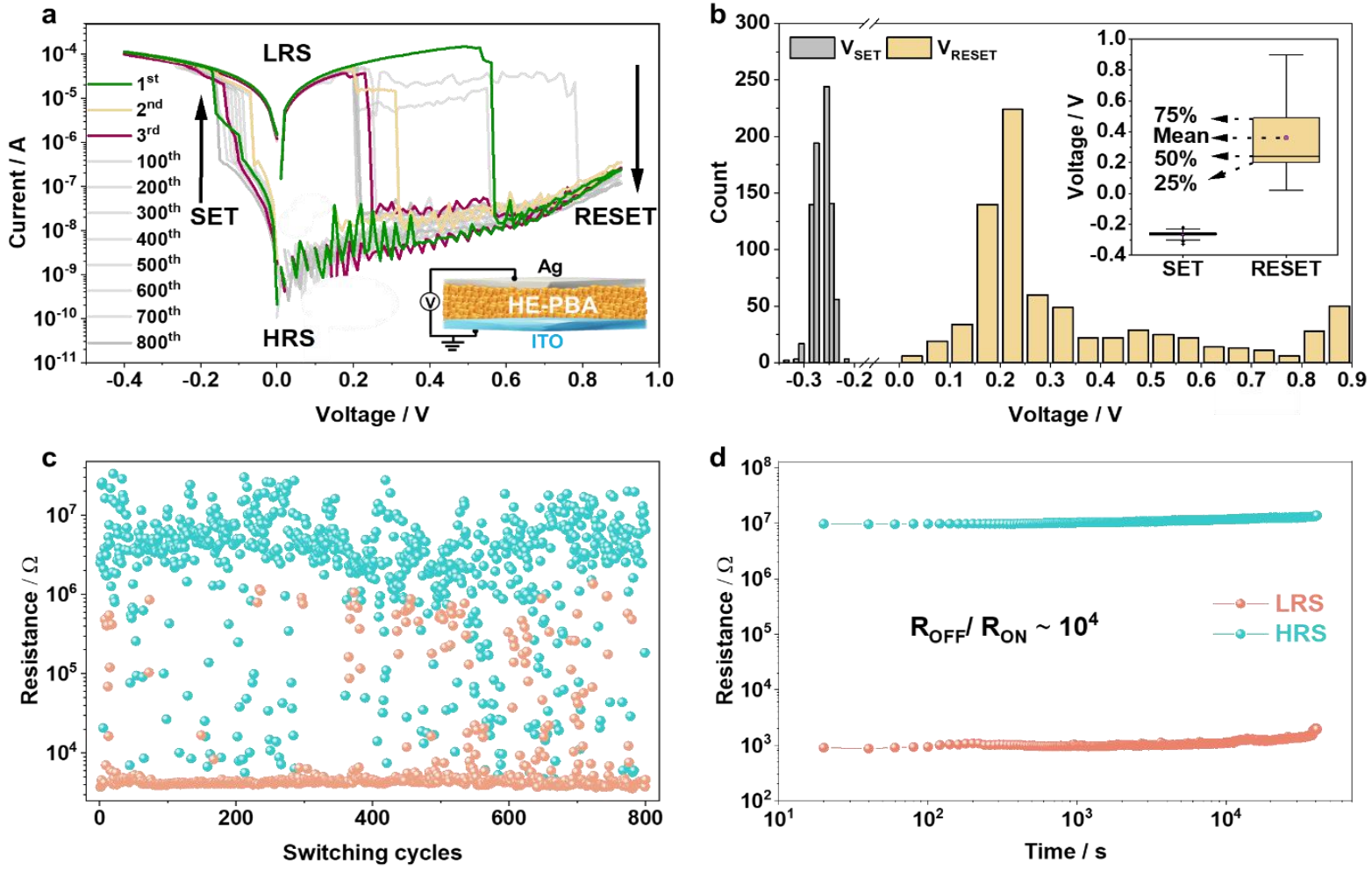


Adv. Mat. 2024, accepted

Electrical Properties of HE-PBA memristor

Measured characteristics

- Bi-polar switching
- No current compliance needed due to self-limitation of current
- Roff/Ron ~10^4
- Low forming voltage 1V
- Good seperation of Set and RESET voltages (0.5V)
- Good retention and endurance mode



Adv. Mat. 2024, accepted

Summary: High Entropy Materials for Information Technology and Energy Devices

Batteries, solar cells, energy applications (Helmholtz Energy, P3T1)

- High-Entropy fluorite-type oxides and tunable band gaps as semi-conductors
- Leveraging Entropy and Crystal Structure Engineering in Prussian Blue Analogue Cathodes for Advancing Sodium-Ion Batteries
- Entropy-Mediated Stable Structural Evolution of Prussian White Cathodes for Long-Life Na-Ion Batteries

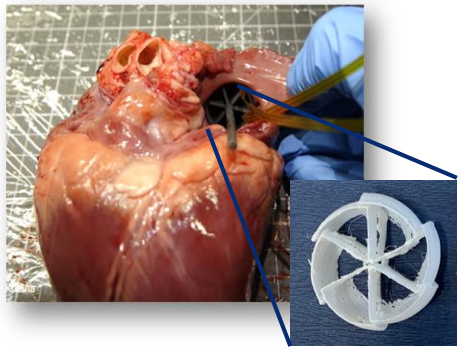
Adv. Energ. Mat. **2023**,13, 2204337, *ACS Nano **2024** 18 (35), 24441,* Angew. Chemie. **2024**, 63 (7), e202315371

Electronic devices with novel materials and manufacturing T1/T2/T3/T5

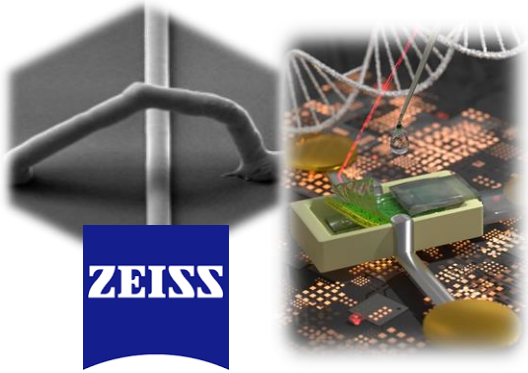
- Review on HEM for energy and electronic applications
- HE-MOF based memristor

*Nat. Rev. Mat. **2024**, 266–281; Adv. Mat. 2024 accepted* , AFM 2024 in rev.

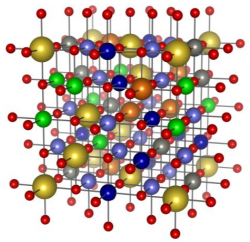
Transfer and Innovation



- **Cooperation with Charité/BIH** on 3D printed prototypes of cardiovascular implants (Left Atrial Appendage Occluder)
- Digitally-designed polymer-based implants (EP 23189962.6) are pursued in a **Start-up strategy**



- **Recent European and US Patent patents in printing technologies**
  - on capillary printed of metallic, superconducting wires and circuits (T1; NACIP)
  - on laser printing of 3D reservoirs with conductive electrodes for bioelectronic applications (T1/T2)
- **Participant in the Zeiss Catalyst Program** on “Liquid metal printing as a deposition method for chiplet technologies”, 2nd and final submission round in December 2024



- **Technology Transfer Project with Hereaus** on HEM for coatings in the semiconductor industry, in particular novel chip technologies, under review by KIT (VP and TT commission), established cooperation within Auto.MAP

Future Perspectives in POFV

Develop Self-Driving-Labs for ..

- technical science applications such as additive manufacturing in photonics and electronics
- sustainable and substitute materials
- new multi-complex materials
- energy applications such as battery materials, catalysts, …

Strengthen ..

- Research and new collaborations on Cluster-based and high entropy materials, neuromorphic materials, devices and bioelectronics across all programs (P3/P2/P1)
- Explore printable quantum devices and circuits within P1/P3