

Materials Science and Technology

### Experimentelle Hochdurchsatzmethoden zur Entwicklung und Charakterisierung neuer Materialien

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# **4 Departements and 4 RFAs**







# **Acceleration of Material Design & Characterization**





NATIONAL CENTRE OF COMPETENCE IN RESEARCH

→ MARVEL targets the accelerated design and discovery of novel materials, via a materials' informatics platform of databasedriven <u>high-throughput</u> quantum <u>simulations</u> Experimental

### Laboratory Automation

- High Troughput Synthesis
- High Througput Analytics
- Robotic Platforms

This Talk: 3 Examples:

- Thin films
- Carbon Nanotubes
- Battery Cells

# Thin films

## **High-throughput experiments for accelerated thin-film development**





We use combinatorial and autonomous sputtering, automated characterization and advanced data analysis to develop advanced deposition processes, **semiconducting thin films**, **piezoelectric** and **ferroelectric** nitrides, **multifunctional** coatings and much more...



#### 3. Automated characterization:

Materials Properties XRD, XRF, 4PP, nano-indentation, UV-Vis, PL, XPS

Materials Durability High-throughput optical aging

#### 4. Advanced Data Analysis:

Automated loading and structuring of data Batch processing & visualization Machine learning for analyzing complex data sets

# Computational prediction of Zn<sub>2</sub>VN<sub>3</sub>

-0.2

-0.4 -0.6

-0.6 1ergy

-1.0 -1.2 -1.2

3

Zn



Selection of material systems:

Down-selection based on requirements



### Zn-V-N phase space:

- Multiple unreported phases
- Zn<sub>2</sub>VN<sub>3</sub> has low formation energy and interesting properties

**DFT calculations:** Formation energies and properties

#### **Material of interest:**

Zn<sub>2</sub>VN<sub>3</sub> a new semiconducting nitride







more information:

S. ZHUK and S. SIOL *et al.* Chem. Mater. 2021 Doi: 10.1021/acs.chemmater.1c03025 S. ZHUK and S. SIOL Appl. Surf. Sci. 2022 Doi: 10.1016/j.apsusc.2022.154172







# **Combinatorial thin-film synthesis**



### Composition / Flux gradients



Temperature gradients



Combinatorial materials libraries



**Combinatorial sputtering:** 

- Thickness or composition gradients
- Temperature gradients can be realized with special heater setups

# **Automated characterization of materials libraries**





characterization and data analysis is critical

Sebastian Siol, 2024

# **Machine learning workflow**



# Products: hardware/software solution



# **Carbon Nanotubes**

### Nanoassembler: Automated process flow for highspeed additive nanostructure assembly & control Manufacturing process overview



Automated CNT Transfer





### High-speed Raman Imaging and Machine Learning Classification

Strategic Focus Area

Advanced Manufacturing









### Automatized Materials Integration Carbon Nanotubes



Automatized, precise positioning & contacting of individual nano-objects

**ETH** zürich

EPEL

https://www.sfa-am.ch/nano-assembly.html

👂 Empa







### **Application example**

Ultra-low power & portable sensors



### **NO<sub>2</sub>** detection demonstrated (sub-ppm level); Benchmarking to manually assembled devices Satterthwaite *et al.,* Sens. Actuator B (2019)

**NB: recovery is accelerated in our case using an external microheater** S. Jung *et al.* Advanced Sensor Research, 3(1), 2300081 (2024) S. Jung *et al.*, Sensors and Actuators B: Chemical, 331, 129406, (2020)



# **Battery Cells**

# Aurora battery assembly and cycling robot



Developed in collaboration with



### Automated coin cell assembly robot

- Assembly of 32 coin cells per batch
- Automated electrode balancing
- Mixing of 32 electrolyte formulations

### Automated coin cell cycling

- 256 dedicated potentiostat channels
- Real-time control of cell cycling parameters
- On-the-fly monitoring of cell cycling data

### Corsin Battaglia, 2024



# Next-generation lithium-ion batteries



- Towards autonomous battery materials discovery
- Robotic platform for automated electrolyte formulation, cell assembly, and cell cycling
- Automated digital workflow and data management infrastructure







https://dgbowl.github.io/

https://big-map.github.io/big-map-registry/apps/aiidalab-aurora.html





- Automated setups to Accelerate Material Development
  - Robotic Platforms for synthesis & Analytics
  - Physics informed Machine Learning
- Broad trend accross domains.