Session of Focus Materialchemie – Wednesday, **24.04.2024** 16:00 – @ Seminarraum Lehar 01 (TU-Wien, Getreidemarkt 9, BC, OG. 01, room A46) – join us on ZOOM (ID: 983 0066 2349)

Development of oxide semiconductor junctions using high-thoughput and machine-learning approaches

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The discovery and optimization of semiconductor materials is a work-intensive and time-consuming task, when relying on conventional experimental routines. The employment of high-throughput techniques speeds up the screening of material properties and facilitates the generation of material libraries for data-driven optimization. In this work, combinatorial deposition is combined with automatized materials characterization and machine-learning approaches.

Ultrasonic spray pyrolysis (USP) is a well-suited technique to create combinatorial thin films, enabling 2D variation of the film composition and/or thickness. Through a gradual composition change of the precursor solution during the deposition process, a 2D gradient of copper-gallium-iron oxides on glass substrates is obtained. The gradient consists of delafossite and wurtzite materials, with a bandgap in the 1-2 eV range, which are highly relevant as earth-abundant light absorbers in photovoltaics and photoelectrochemical water splitting. Automatized, spatially resolved SEM/EDS, FTIR, and XRD measurements reveal the combinatorial capabilities of the developed process.

The former methods enable valuable insights into semiconductor materials; however, the optoelectronic properties of the intended heterojunctions are highly relevant as well. To this end, a platform for combinatorial device characterization is developed, designed to measure a matrix of 8x8 individual cells on a single sample of 25x25 mm² size. The corresponding Python package facilitates the automatized measurement by providing a modular framework for the integration of sample designs, measurement instruments, and characterization routines. Using this platform, a screening for the optimum Ga_2O_3 film thickness in heterojunctions with sputtered Cu_2O is performed using only 3 samples. Furthermore, leveraging its built-in statistical strength, a machine learning backed investigation of all-sprayed Ga_2O_3-Cu_2O is conducted. The USP process parameters for the deposition of Cu_2O are optimized, relying on Latin Hypercube Sampling and Bayesian Optimization.

In summary, this work presents a comprehensive approach combining combinatorial deposition, automated materials characterization, and machine learning techniques to accelerate the discovery and optimization of semiconductor materials, paving the way for efficient exploration of optoelectronic