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COHESIVM: Combinatorial h+/e- Sample Investigation using Voltaic Measurements

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Software

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Summary

Accelerating materials discovery and optimization is crucial for transitioning to sustainable energy conversion and storage. In this regard, materials acceleration platforms (MAPs) can significantly shorten the discovery process, cutting material and labor costs (Aspuru-Guzik & Persson, 2018). Combinatorial and high-throughput methods are instrumental in developing said MAPs, enabling autonomous operation and the generation of large datasets (Maier et al., 2007). Therefore, in a previous work, we developed combinatorial deposition and analysis techniques for the discovery of new semiconductor materials (Wolf et al., 2023). To drive further innovation in the field, COHESIVM was created, which facilitates combinatorial analysis of material and device properties through the following key features:

- A **generalized workflow** reduces redundancy and ensures consistency across different experimental setups.
- The **modular design** abstracts devices, contact interfaces, and measurement routines into interchangeable units.
- **Efficient data handling** is achieved through robust metadata collection and well-structured storage.

Statement of need

COHESIVM is a Python package that aims to streamline the setup and execution of combinatorial voltaic measurements. Typically, experimental workflows and data handling are implemented on a use-case basis, which can be time-consuming and error-prone. With COHESIVM however, these foundational features are pre-implemented and designed to be reusable across different scenarios. The package provides a generalized framework, following well-documented abstract base classes, which facilitates the implementation of application-specific components. Additionally, graphical user interfaces allow users with less programming experience to execute experiments and analyze the collected data.

COHESIVM stands out for its straightforward design and the ease with which it can be interfaced with existing APIs to implement new devices seamlessly. While there are a number of tools available in the public domain that provide control over measurement equipment (Fuchs et al., 2024; Pernstich, 2012; Weber, 2021), many of these tools focus primarily on graphical user interfaces which can limit their flexibility. Python APIs, such as `bluesky` (Allan et al., 2019), do offer experiment control and data collection capabilities. However, COHESIVM's advantage lies in its simplicity and targeted application in combinatorial experiments.

For the investigation of combinatorial optoelectronic devices, COHESIVM includes hardware descriptions as well as implemented components which enable to quickly screen a matrix of

8 × 8 pixels on a single substrate (25 mm × 25 mm). The package's documentation provides a high-level description of how COHESIVM can be applied in this context. In brief, 64 gold pads are sputtered onto the sample using a mask which is available in the repository. Schematics and board files for reproducing the utilized `MA8X8` interface are provided as well. After mounting the sample on this interface, it is placed under a solar simulator (Ossila, AAA classification) and connected to the electronic measurement equipment (Agilent 4156C). Employing the `CurrentVoltageCharacteristic` measurement class, the IV curves of all 64 pixels are recorded and the resulting data yields a map of open-circuit voltages.

Author Contributions

Maximilian Wolf: Methodology, Software, Writing - Original Draft. **Selina Götz:** Software, Validation. **Georg K.H. Madsen:** Writing - Review & Editing, Supervision. **Theodoros Dimopoulos:** Conceptualization, Resources, Supervision.

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