Conjugated Polymer Process Ontology and Experimental Data Repository For Organic Field Effect Transistors

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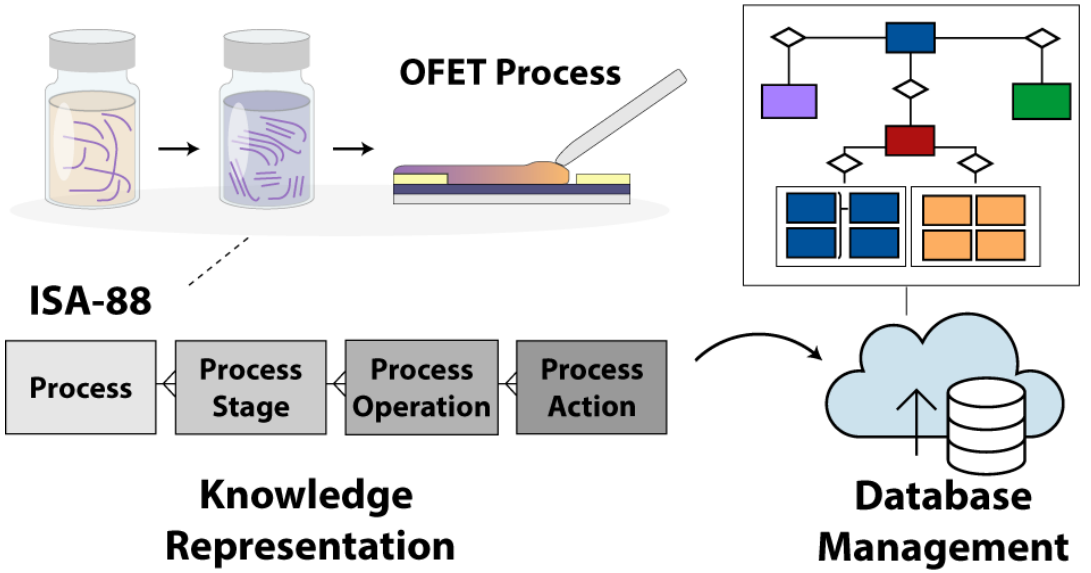
Polymer-based semiconductors offer great potential for informatics-driven organic electronics research. However, the complex processing space coupled with sparse experimental details hinder data-driven analysis. To address these issues, we have developed and put into practice an object-relational database for storing experimental records of OFETs and enable data-driven discovery.

- The ISA-88 standard was used to design a robust data structure for systematically storing and analyzing representative OFET data records
- Data ontologies that comprehensively describe sample origin and processing history were proposed, and their adoption to improve standards within the community was recommended
- ~500 OFET data records from literature and lab experiments were integrated into the database, enabling data-driven analysis of process-structure-property relationships

This work paves the way for widespread adoption of data management practices and design standards in the organic electronics field and materials community.



A. L. Liu, M. Lee et al., Conjugated Polymer Process Ontology and Experimental Data Repository for Organic Field Effect Transistors, Chem. Mater. 2023, (https://doi.org/10.1021/acs.chemmater.3c01842)

Collaboration with UIUC to Develop Online Database Knowledge Platform for Organic Thin Film Electronics

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The DMREF team collaborated with Dr. Ying Diao from the University of Illinois Urbana-Champaign (UIUC) to create an online database knowledge platform for organic electronic devices. This platform will enable researchers in the community to access and contribute experimental data on organic field-effect transistors (OFETs) through a web interface. The proposed interface will also include data visualization and analysis tools, allowing users to explore the data and gain insights.

4 undergraduate students were recruited for the project :

- A student at Georgia Tech recruited as part of the Summer Undergraduate Research in Engineering/Sciences (SURE) program helped develop the front end for the user interface
- A student at Lehigh recruited under a Summer Experiential Learning Fellowship helped with data curation and database development activities
- A student at UIUC recruited from the computer science department helped with front end development
- A second student at Georgia Tech recruited from computer science department helped with back-end development

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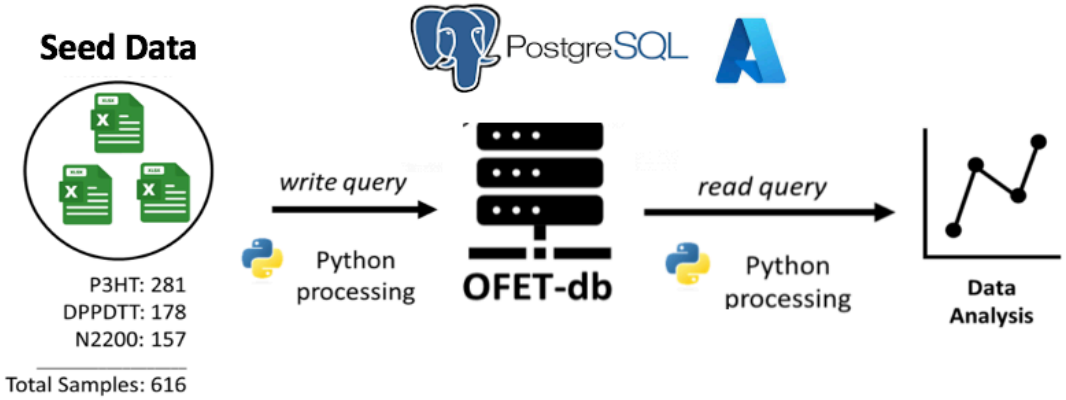

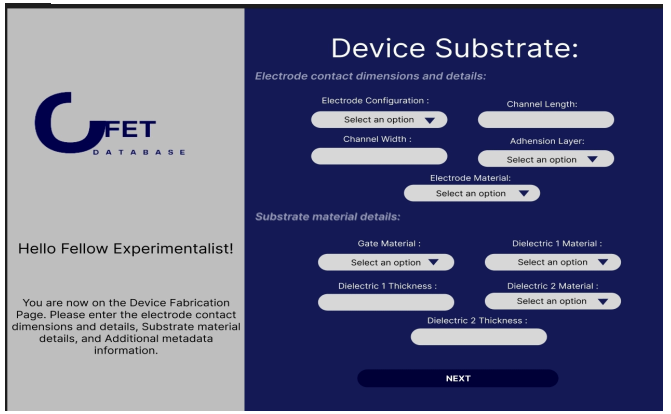

Figure. (left) OFET-DB Data curation pipeline. 600 OFET devics were curated and inserted into a PostgreSQL based database hosted on an azure cloud server. (below) User interface to interact with the database and add OFET experimental data.

Chain Conformation, Exciton Delocalization and Dynamics in a Push-Pull Conjugated Polymer

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The DMREF team recently published a peer-reviewed article that discusses possible correlations between chain conformation, and exciton delocalization and dynamics by studying the linear and nonlinear optical lineshape along with corresponding solution-viscosity measurements.

- Absorption, photoluminescence and transient absorption spectroscopies were implemented in the electron push-pull polymer DPP-DTT, to explore the relationship between spectral lineshape and chain conformation deduced from resonance Raman spectroscopy and *ab initio* calculations.
- The exciton appeared more dispersed along the polymer chain backbone with increasing polymer solution concentration and also exhibited strong interchain coupling.

Thus, tuning the microscopic chain conformation by concentration is a factor of interest when considering polymer assembly pathways for the pursuit of large-area, high-performance organic optoelectronic devices.

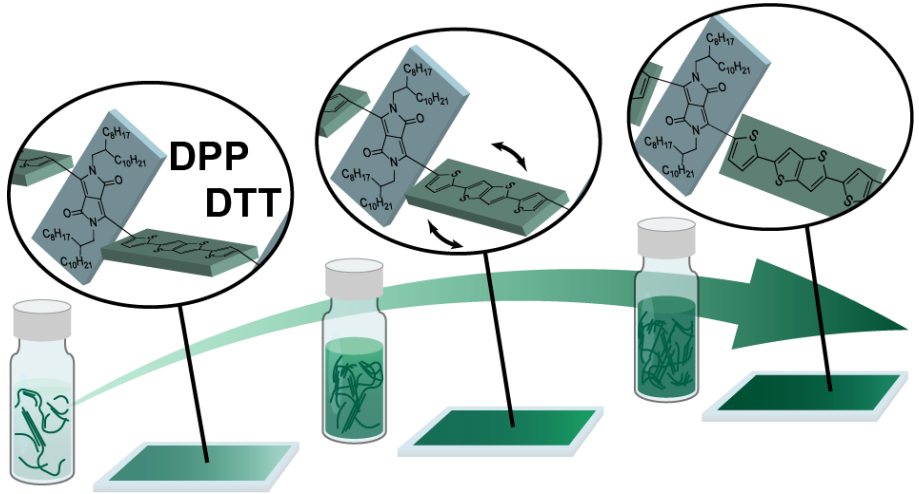

Figure. Schematic of chain conformation in thin films transforms with increasing precursor solution concentration

Zheng Y., Venkatesh, R. *et al.*"Exciton Delocalization and Chain Conformation in a Push-Pull Conjugated Polymer." arXiv. 2303.10927, Chemistry of Materials 2023, Accepted.