Open-Hardware Materials Acceleration Platforms for Accessible and Democratized Materials Discovery

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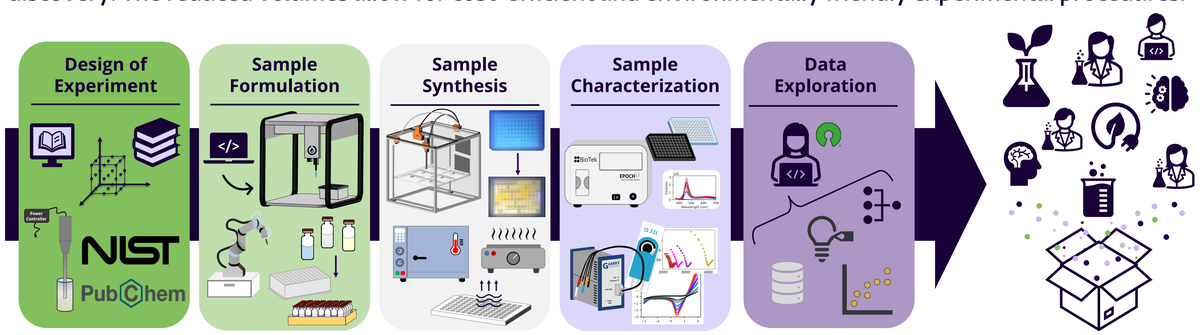
Low-cost and open-hardware based materials acceleration platforms (MAPs), implementing commercially available materials, and adopting open-science principles enable more accessible and affordable materials discovery. The reduced volumes allow for cost-efficient and environmentally friendly experimental procedures.

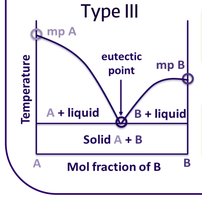


High-Throughput and Data Driven Strategies for the Design of Deep-Eutectic Solvent Electrolytes

Background

Deep Eutectic Solvents:
Mixture of 2 compound with T_m lower than that of the starting material

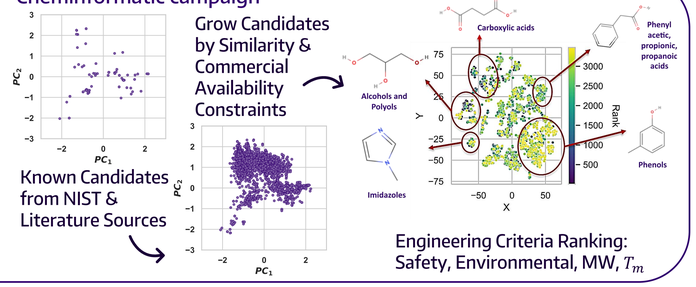
Type III



Quaternary Ammonium Salt (QAS) + Molecular Hydrogen Bond Donor (HBD)

low toxicity, low flammability, commercial availability, low costs → Large design space largely unexplored → Need for fast & systematic characterization

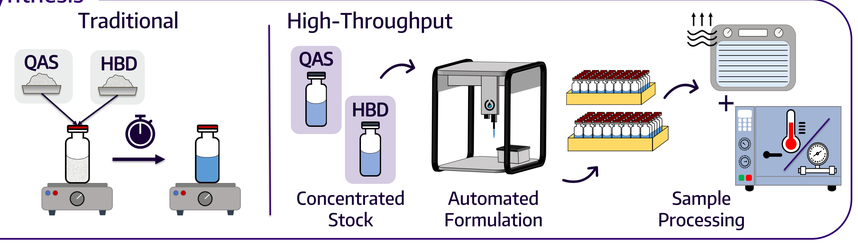
Cheminformatic campaign



Engineering Criteria Ranking: Safety, Environmental, MW, T_m

Traditional vs. High-Throughput Synthesis

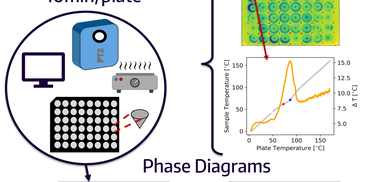
Experimental Design	
	5 QAS & 10 HBD
	12 Concentrations
	600 samples
	0.6 mL total volume/sample
	4 weeks experimental campaign



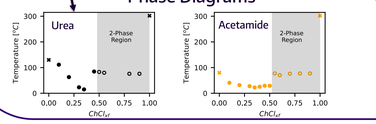
Results

T_m Determination- PhasIR

- 48+ samples at a time
- ~10min/plate



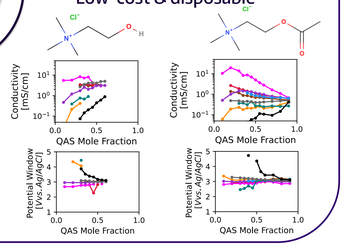
Phase Diagrams



Electrochemical Testing

- Carbon CE-WE & Ag/AgCl RE
- 100 µL/sample
- ~ 7 min/sample
- Low-cost & disposable

Ionic Conductivity



Potential Window

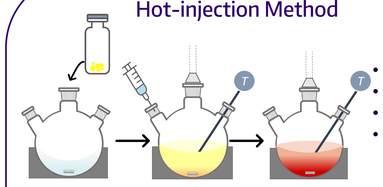
Conclusion

- The cheminformatics approach resulted in 3,477 HBD and 185 QAS
- 600 unique samples were synthesized
- 230 samples were found to be liquid at room temperature
- Several DES with conductivities above 1 mS/cm
- Nearly all DES samples showed stable potential windows greater than 3 V

High-Throughput Workflow for the Synthesis of CdSe Nanocrystals Using a Sonochemical Materials Acceleration Platform

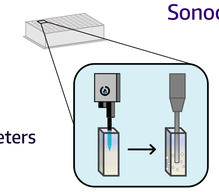
Traditional vs. High-Throughput Synthesis

Hot-injection Method



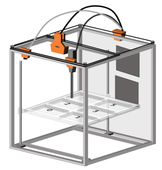
- Complex experimental conditions
- Difficult to scale
- Prone to human variability
- Only a single combination of parameters

Sonochemical Synthesis



- One-pot synthesis
- Scalable
- Ambient experimental conditions
- Allows for formation of magic-sized (<2 nm) QD intermediates

Experimental Design	
	4 Different Components
	5 Concentrations
	625 samples – *in triplicate*
	0.5 mL total volume/sample
	5 minutes of (active) sonication



Sonication Station

- Repurposed 3D printer platform (Jubilee)
- Customizable Automated protocols
- Open-Source/ Open-Hardware
- Various applications: sonochemical synthesis, emulsions, etc.

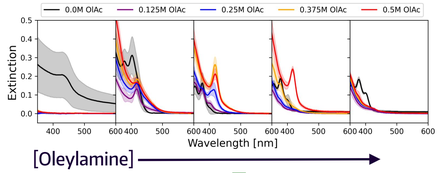
Synthesize, Process, Characterize **1875 samples**

Traditional Route: > 1 year

MAPs: < 6 weeks

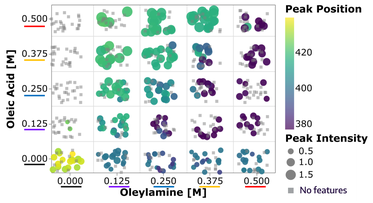
Results & Visualization Challenges – UV-Vis

0.1 M CdAc & 0.1 M Se

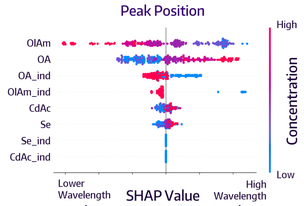


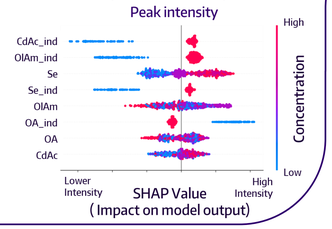
[Oleylamine]

All 625 conditions



Model-Agnostic Interpretation Method: SHAP





2D representation of spectra only visualizing 25 conditions at a time

By extracting feature from the UV-Vis spectra, we can start comparing all experimental conditions

SHAP Analysis confirms the trends of all variables tested.

Conclusion

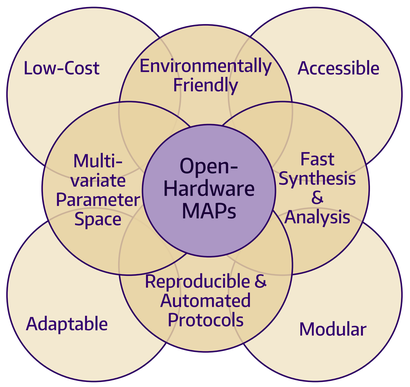
- Oleylamine promotes nucleation of small QDs in low concentrations
- Oleic Acid promotes the formation of large QDs in higher concentrations

Analogous analysis for Fluorescence data showed:

- Oleylamine promotes high intensity emissions
- Oleic Acid leads to surface trap emission behavior
- Unreacted ligands cause scattering below 500 nm

Take-Aways

- We demonstrated two high-throughput workflows based on open-hardware MAPS (<$15k) for the exploration of soft matter systems involving large chemical design spaces.
- The combination of MAPs with data-driven strategies allows for faster material discovery
- The flexibility, modular nature, and reconfigurability of these high-throughput platforms, makes them adaptable to a variety of soft matter formulation studies



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